Temporal control in tritylation reactions through light-driven variation in chloride ion binding catalysis – A proof of concept

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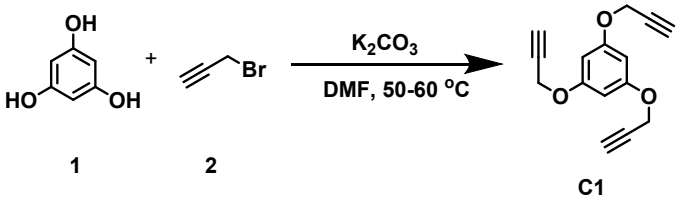
S1. General methods:

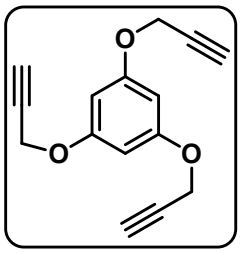
All the reactions have been carried out using the oven dried glasswares. The reagents (AR grade or LR grade) and solvents have been purchased from commercially available sources such as Sigma-Aldrich, Merck, Himedia, Rankem, CDH, TCI, Alfa Aesar etc. Anhydrous solvents for the reactions and for column chromatography have been distilled before use. Column chromatography was performed over silica gel (100–200 mesh) using EtOAc/hexane and DCM/MeOH as an eluent. Thin layer chromatography was performed on Merck Silica gel 60 F_{254} TLC plates and visualized using UV (λ = 254 nm) chamber or iodine stain. Melting points were recorded on SMP20 melting point apparatus and were uncorrected. IR spectra for all the samples were recorded using a Bruker Alpha ZnSe ATR or Perkin Elmer Spectrum Two FTIR spectrometers at 4 cm^{-1} resolution. The NMR spectra have been recorded in Bruker Avance-III 400 MHz spectrometer. ^{1}H and ^{13}C NMR were recorded at operational frequencies 400 MHz and 100 MHz, respectively. For recording NMR spectra, $CDCl_3$ and DMSO-d_6 have been used as the solvents, and the residual solvent signals have been used for calibration. The chemical shift (δ) values are reported in parts per million (ppm) and the coupling constants (*J*) are reported in Hz. High resolution mass spectra (HRMS) have been recorded using Waters Synapt G2-Si Q-TOF mass spectrometer. HRMS data were obtained from a TOF mass analyser in both positive and negative modes using either electrospray ionization (ESI) or Matrix-assisted laser desorption/ionization (MALDI) methods. The electronic absorption spectra were recorded using a Cary 5000 UV-Vis-NIR spectrophotometer or Cary 60 UV-Vis spectrophotometer. Commercially available UV (Nichia 365 nm) LED, Applied Photophysics with different wavelengths of LEDs, and 405 nm LED light sources have been used for the forward and reverse photoisomerisation processes and screening of irradiation wavelengths. Isothermal titration calorimetry (ITC) experiments were performed using Malvern MicroCal PEAQ-ITC200.

S2. Synthesis:[1-8]

S2.1 Synthesis of core unit C1:[1]

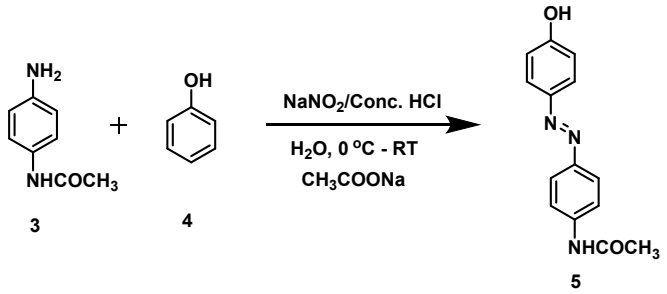


To a solution of phloroglucinol **1** (1.26 g, 10 mmol) in dry DMF (30 mL), anhydrous potassium carbonate (5.52 g, 40 mmol) was added and heated to 50 °C for 1 h under nitrogen atmosphere. Propargyl bromide **2** (4.76 g, 40 mmol) was then dropwise added and the reaction was continued at 65 °C for 36 h. After completion, the reaction mixture was cooled down to room temperature, and was poured into water. The crude solid product was collected by filtration. The pure product was obtained as fine white needle crystals after purification by column chromatography.

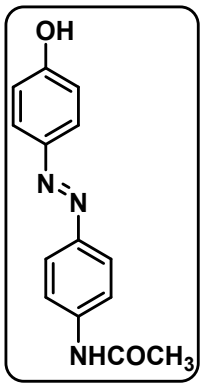


1,3,5-*tris*(prop-2-yn-1-yloxy)benzene (**C1**): White solid, mp= 82-84 °C, 57% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 6.25 (s, 3H), 4.75 (d, J = 2.4 Hz, 6H), 3.57 (t, J = 2.3 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 158.9, 95.1, 79.1, 78.4, 55.6; FT-IR (KBr): 3279, 3269, 3259, 2908, 2134, 2115, 1617 cm^{-1}.

S2.2.1a Synthesis of *(E)*-N-(4-((4-hydroxyphenyl)diazenyl)phenyl)acetamide(5):[2]

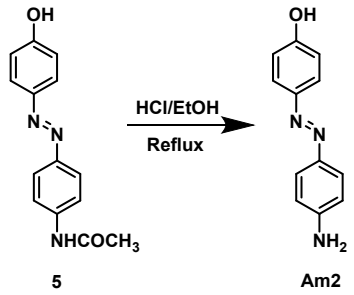


In a round bottom flask, 4-aminoacetanilide **3** (3.3 g, 22 mM) was dissolved in deionized water and the flask was cooled to 0 °C. To this mixture, 37% conc. HCl (6.5 mL) was added. Then a cold aqueous solution of sodium nitrite (1.52 g, 22 mM) in 20 mL of water was dropwise added into the reaction mixture. After the addition, the reaction mixture was allowed to stir for half an hour. Afterwards, cold aqueous solutions of sodium acetate (5.9 g, 70 mM) and phenol **4** (2.16 g, 23 mM) in 100 mL of water were sequentially added at 0 °C. After the addition, the reaction was allowed to stir at RT and was monitored by TLC. After completion of the reaction, the reaction mixture was filtered off and water washings were given to obtain the pure orange solid product, which was dried under vacuum.

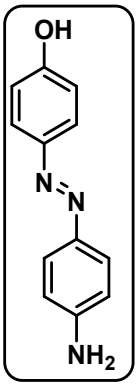


(E)-N-(4-((4-hydroxyphenyl)diazenyl)phenyl)acetamide(**5**): Dark orange solid, mp= 157-160°C, 91% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 10.29 (s, 1H), 7.77-7.73 (m, 6H), 6.92 (d, J = 8.4 Hz, 2H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 168.8, 161.1, 147.7, 145.2, 141.5, 124.6, 123.1, 119.2, 116.1, 24.2; FT-IR (ATR): 3341, 3043, 2998, 2920, 2789, 2660, 2586, 1651, 1587, 1529, 1500, 1401,1369, 1322, 1264,1226, 1142, 965, 834, 675, 640cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{14}H_{13}N_3O_2[M+H]^+$: 256.1088; found : 256.1086.

S2.2.1b Synthesis of (*E*)-N-(4-((4-hydroxyphenyl)diazenyl)phenyl)acetamide(Am2):



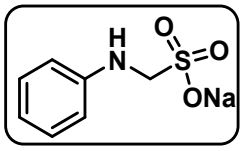
To the (*E*)-N-(4-((4-hydroxyphenyl)diazenyl)phenyl)acetamide **5** (1.75 g, 5.16 mM) in ethanol (150 mL), 37% con. HCl (4 mL) was added and refluxed. The hydrolysis reaction was monitored by TLC. After completion of the reaction, the reaction mixture was neutralised by adding aqueous sodium bicarbonate solution. The extraction of the reaction mixture was done using ethyl acetate. The extracted organic layer was washed with brine solution and evaporated to dryness and was subjected to purification by column chromatography.



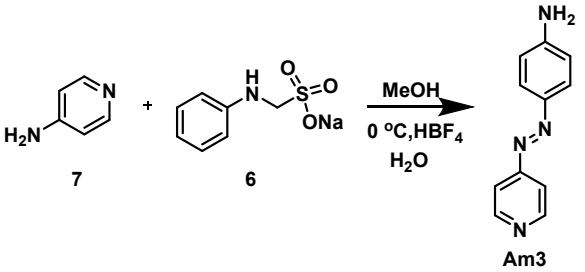
(*E*)-4-((4-aminophenyl)diazenyl)phenol (**Am2**): Orange solid, mp= 185-190 °C, 88% yield. ^{1}HNMR (400 MHz, DMSO-d_6): δ (ppm) 9.98 (d, J = 6.9 Hz, 1H), 7.66-7.56 (m, 4H), 6.87 (t, J = 8.0 Hz, 2H), 6.64 (t, J = 7.7 Hz, 2H), 5.89 (br, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 159.2, 151.9, 145.6, 142.9, 124.5, 123.7, 115.8, 113.5; FT-IR (ATR): 3359, 3286, 3004, 2672, 1589, 1493, 1470, 1448, 1385, 1238, 1150, 1143, 1099, 1095, 1088, 1007, 948, 883, 836, 804, 762, 728, 710 cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{12}H_{11}N_3O[M+H]^+$: 214.0980; found : 214.0971.

S2.2.2 Synthesis of sodium (phenylamino)methanesulfonate(6):[3]

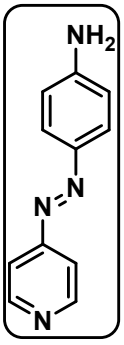
To a solution of formaldehyde (0.1 mol) and distilled water (40 mL), sodium bisulfite (0.1 mol) was added with stirring. The mixture was heated to 65 °C for 1 h. To this mixture, aniline (0.08 mol) was dropwise added over 15 min and stirred for 2 h at 65 °C. The reaction mixture was cooled to about 0 °C, which resulted in a dull-white crystalline solid that was filtered off, which was dried and used directly for next step.



S2.2.3 Synthesis of (*E*)-4-(pyridin-4-yldiazenyl)aniline Am3:[4]

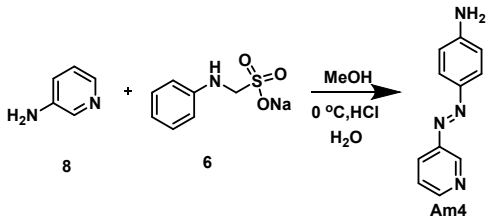


4-Aminopyridine **7** (0.500 g, 5.3 mmol) was dissolved in 20 ml of 85% aqueous fluoroboric acid solution and cooled to 0 °C. To this, 0.296 g of sodium nitrite was slowly added while maintaining the temperature below 5 °C. After stirring for about one hour, 2.208 g of sodium (phenylamino)methanesulfonate**6** as a suspension in 30 ml cold methanol was dropwise added, while maintaining the internal temperature below 5 °C. After the addition, the reaction mixture was warmed to room temperature, and 20 ml of isopropanol was dropwise added to it. The product as a precipitate filtered off to give wet crystals. This product was dissolved in 0.269 g of sodium hydroxide in 32ml of water and refluxed for 1-2 hours. After cooling down to room temperature, an orange solid product was filtered off, washed with acetonitrile and dried.

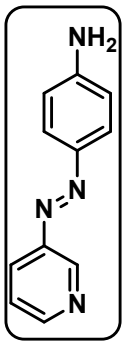


(*E*)-4-(pyridin-4-yldiazenyl)aniline(**Am3**): Orange solid, 90% yield. ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 8.74-8.73 (dd, J = 4.6, 1.6 Hz, 2H), 7.85 (d, J = 8.8 Hz, 2H), 7.64 (dd, J = 4.6, 1.6Hz, 2H), 6.75 (d, J = 8.8 Hz, 2H), 4.22 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 151.2, 151.1, 146.5, 145.5, 126.2, 116.2, 114.7; FT-IR (ATR): 3435, 3301, 3139, 1639, 1600, 1587, 1504, 1456, 1416, 1400, 1320, 1136, 839 cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{11}H_{10}N_4$ $[M+H]^+$: 199.0983; found : 199.0981.

S2.2.4 Synthesis of (*E*)-4-(pyridin-3-yldiazenyl)aniline (Am4):[4]

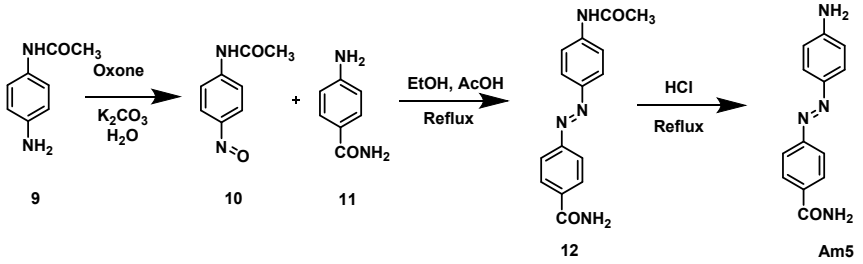


3-Aminopyridine **8** (0.500 g, 5.3 mmol) was dissolved in 5 ml of 37% hydrochloric acid, and cooled to 0 °C. To this, 0.296 g of sodium nitrite as aqueous solution (5 mL) was dropwise added slowly while maintaining the temperature below 5 °C. The reaction mixture was stirred for about one hour. Afterwards, 2.208 g of sodium (phenylamino)methanesulfonate**6**as a suspension in 30 ml cold methanol was dropwise added slowly, while maintaining the internal temperature below 5 °C. After the addition, the reaction mixture was warmed to room temperature, and 20 ml of isopropanol was dropwise added in to it. The product as a precipitate was filtered off to give wet crystals. This product was dissolved in aq. sodium hydroxide solution (0.269 g of sodium hydroxide in 32ml of water), and refluxed for 1-2 hours. After cooling to room temperature, the product was filtered off, washed with acetonitrile and dried.



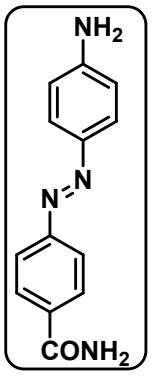
(*E*)-4-(pyridin-3-yldiazenyl)aniline (**Am4**): Orange solid, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm)9.104-9.098 (m, 1H), 8.62-8.61 (dd, J = 4.7, 1.6 Hz, 1H), 8.09-8.06 (ddd, J = 8.2, 2.3, 1.6 Hz, 1H), 7.84-7.81 (m, 2H), 7.41-7.38 (ddd, J = 8.2, 4.8, 0.6 Hz, 1H), 6.76-6.72 (m, 2H), 4.17 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm)150.6, 150.4, 148.4, 146.9, 145.6, 126.7, 125.7, 123.9, 114.7;FT-IR (ATR): 3368, 3328, 3151, 1660, 1601, 1571, 1384, 1332, 1138, 824, 703 cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{11}H_{10}N_4[M+H]^+$: 199.0983; found : 199.0982.

S2.2.5 Synthesis of (*E*)-4-((4-aminophenyl)diazenyl)benzamide (Am5):



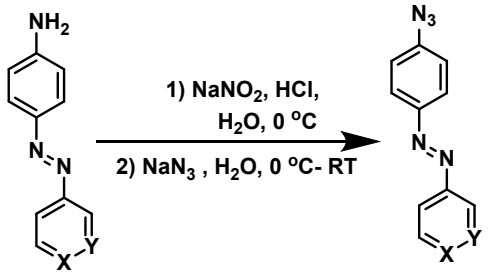
In a round bottom flask, aqueous solution of oxone (4.6 eq., 9.4 g) with K_2CO_3 (2.6 eq., 2.4 g) was taken and stirred at room temperature. To this, an aqueous solution of 4-aminoacetanilide **9** (1 eq., 1 g) was quickly added. A green solid product of nitroso compound **10** was obtained, which was filtered off after half an hour. The wet solid product was directly utilised for the next step. Mill's method was adopted for a condensation reaction between the crude nitroso compound **10** formed in first step (1 eq, 1.068 g) and 4-aminobenzamide **11** (1 eq, 0.976 g). This was performed by refluxing these reactants in EtOH (10 ml) and acetic acid (5 ml) for 7 hrs and monitored by TLC. After

completion of the reaction, the hydrolysis step was continued by refluxing the *in situ* generated amide product **11** under conc. HCl condition for 3 hrs. After completion of the reaction, the reaction mixture cooled down to room temperature and was neutralised by adding aqueous sodium bicarbonate solution. The product was extracted using ethyl acetate, the organic layer was washed with brine solution, and evaporated to dryness. The crude product was then subjected to purification by column chromatography.



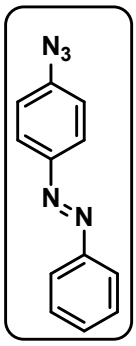
(*E*)-4-((4-aminophenyl)diazenyl)benzamide (**Am5**): Orange solid, 97% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 8.08 (s, 1H), 7.99 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.7 Hz, 2H), 7.45 (s, 1H), 6.68 (d, J = 8.7 Hz, 2H), 6.25 (s, 2H); ^{13}C-NMR (100 MHz, DMSO-d_6): δ (ppm) 167.6, 154.2, 153.5, 143.0, 134.4, 128.7, 125.8, 121.5, 113.6; FT-IR (neat): 3392, 3327, 3233, 2919, 1697, 1593, 1422, 1269, 1136, 1094 cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{13}H_{12}N_4O[M+H]^+$: 241.1089; found : 241.1079

S2.2.6 Synthesis of 4-azido azoarene and azoheteroarene derivatives[5]

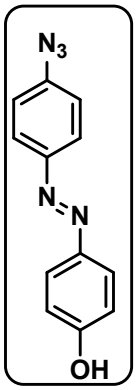


Am1-5 **Az1-5**

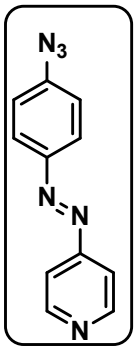
General Procedure: In a round-bottom flask, amines **Am1-5** (10 mmol) was dissolved in HCl (6 N, 10 mL) in an ice bath. $NaNO_2$ (15 mmol) dissolved in 25 mL water was dropwise added. The reaction mixture was stirred for 30 min. Sodium azide (40 mmol) dissolved in 50 mL water was dropwise added. Afterwards, the reaction mixture was stirred for another 2–4 hours at room temperature and followed by TLC. Then, the mixture was extracted with ethyl acetate and the combined organic extracts were washed with H_2O, dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo and then subjected to purification by column chromatography using neutral alumina.



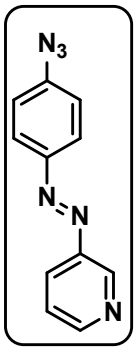
(*E*)-1-(4-azidophenyl)-2-phenyldiazene (**Az1**): Orange solid, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.95 (d, J = 8.3 Hz, 2H), 7.90 (d, J = 7.9 Hz, 2H), 7.54-7.46 (m, 3H), 7.16 (d, J = 8.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm)152.7, 149.9, 142.7, 131.2, 129.3, 124.7, 122.9, 119.7; FT-IR (ATR): 2922, 2115, 1593, 1579, 1494, 1287, 1129, 838, 764, 687,543 cm^{-1}.



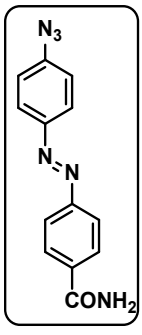
(*E*)-4-((4-azidophenyl)diazenyl)phenol (**Az2**): Orange solid, 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm)7.89 (d, J = 8.3, 2H), 7.86 (d, J = 8.4 Hz, 2 H), 7.14 (d, J = 8.3 Hz, 2H), 6.95 (d, J = 8.3 Hz, 2H), 5.63 (s, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$): δ(ppm)159.1, 150.0, 146.9, 142.0, 125.1, 124.4, 119.7, 116.0; FT-IR (ATR): 3424, 2403, 2252, 2115, 1587, 1579, 1471, 1442, 1413, 1386, 1299, 1286, 1223, 1152, 1143, 1129, 1107, 1005, 944, 839, 813, 808, 773, 726, 709, 670 cm-1; HRMS (ESI): *m/z* calcd. for $C_{12}H_9N_5ONa[M+Na]^+$: 262.0705; found : 262.0703.



(*E*)-4-((4-azidophenyl)diazenyl)pyridine (**Az3**): Orange solid, 97% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 8.81-8.80 (dd, J = 4.6, 1.6 Hz, 2H), 8.01-7.98 (m, 2H), 7.71-7.69 (dd, J = 4.6, 1.6, 2H), 7.20-7.16 (m, 2H); ^{13}C-NMR (100 MHz, DMSO-d_6): δ (ppm) 157.2, 151.5, 149.6, 144.3, 125.4, 119.9, 116.4; FT-IR (ATR): 2975, 2935, 2134, 2110, 1617, 1471, 1450, 1369, 1272, 1157, 1062, 1015, 975, 956, 950, 909, 814. cm^{-1};HRMS (ESI): *m/z* calcd. for $C_{11}H_8N_6$ [M+Na]$^+$: 247.0708; found : 247.0710.

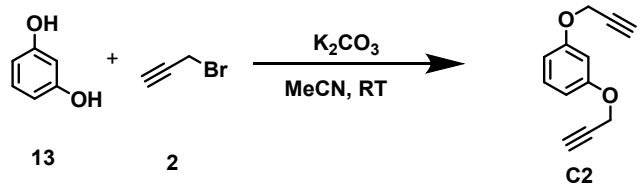


(*E*)-3-((4-azidophenyl)diazenyl)pyridine (**Az4**): Orange solid, 95% yield.^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 9.17 (d, J = 2.1 Hz, 1H), 8.70-8.68 (dd, J = 4.7, 1.5 Hz, 1H), 8.14-8.11 (ddd, J = 8.2, 2.2, 1.6 Hz, 1H), 7.99-7.95 (m, 2H), 7.46-7.42 (ddd, J = 8.2, 4.8, 0.6 Hz, 1H), 7.18-7.15 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 151.8, 149.7, 147.9, 147.5, 143.6, 126.9, 125.0, 124.1, 119.8; FT-IR (ATR): 2920, 2115, 1566, 1486, 1254, 1091, 1023, 834 cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{11}H_8N_6Na$ [M+Na]$^+$: 247.0708; found : 247.0710.



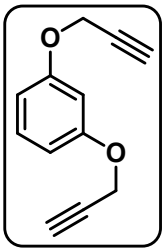
(*E*)-4-((4-azidophenyl)diazenyl)benzamide(**Az5**): Orange solid, 90% yield.^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 8.21-8.18 (m, 2H), 8.00-7.96 (m, 2H), 7.95-7.92 (m, 2H), 7.19-7.15 (m, 2H);^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 166.1, 155.0, 149.7, 143.4, 132.1, 130.6, 125.0, 122.6, 119.7; FT-IR (ATR): 3451, 3185, 2924, 2132,1660, 1596, 1396, 1278, 1123, 863 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{11}H_8N_6Na$ [M+Na]$^+$: 247.0708; found : 247.0710.

S2.2.8 Synthesis of core unit C2:[6]



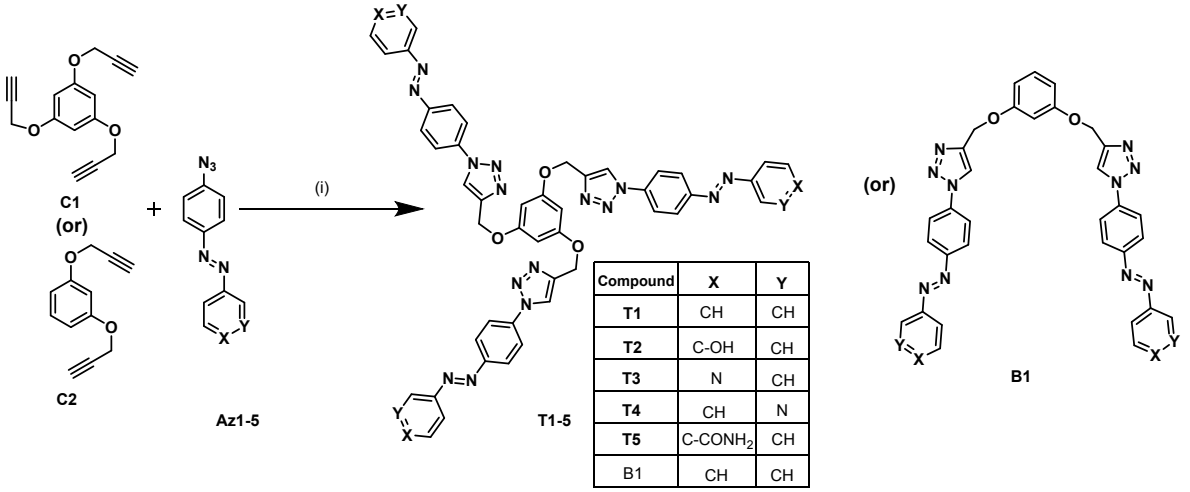
13 2 C2

A mixture of resorcinol **13** (1 g, 9.09 mmol) and anhydrous potassium carbonate (5.01 g, 36.4 mmol) in dry acetonitrile (30 mL), was refluxed for 1h and then propargyl bromide **2** (4.37 g, 36.4 mmol) was added to it. The reaction mixture was further refluxed for 4h. After completion of the reaction, the organic solvent was evaporated off under reduced pressure and water was added to it. The reaction mixture was then extracted with $CHCl_3$, washed with water and dried over anhydrous Na_2SO_4. Evaporation of the solvent gave the crude product, which was purified by column chromatography using hexane and ethylacetate as the eluent.



1,3-*bis*(prop-2-yn-1-yloxy)benzene (**C2**): Colourless liquid, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.24-7.19 (m, 1H), 6.62 (d, J = 6.3 Hz, 3H), 4.66 (s, 4H), 2.54 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 158.7, 130.0, 107.9, 102.4, 78.5, 75.7, 55.9.

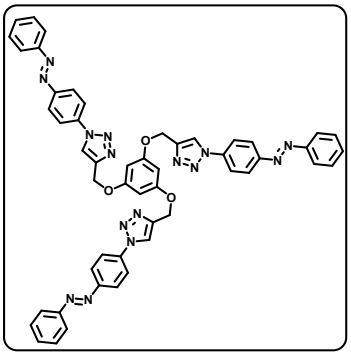
S2.2.8Synthesis of catalysts T1-5 and B1:[7]



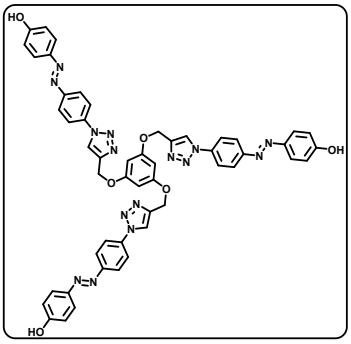
Compound	X	Y
T1	CH	CH
T2	C-OH	CH
T3	N	CH
T4	CH	N
T5	C-$CONH_2$	CH
B1	CH	CH

General Procedure: For click chemistry,1,3,5-*tris*(prop-2-yn-1-yloxy)benzene **C1**(1.0 eq for **T1-5**) or 1,3-*bis*(prop-2-yn-1-yloxy)benzene **C2**(1.0 eq for **B1**) was added with the corresponding azides**Az1-5** (3.3 eq for **T1-5** and 2.2 eq. for **B1**) in 5 ml of 1:1 ^{t}BuOH/H_2O mixture. Followed by, the $CuSO_4.5H_2O$ (0.6 eq) and sodium ascorbate (1.2 eq) were added as an aqueous solution. The reaction was stirred for 3 days at room temperature and followed by TLC. The resulting yellow coloured precipitate was filtered off and was washed

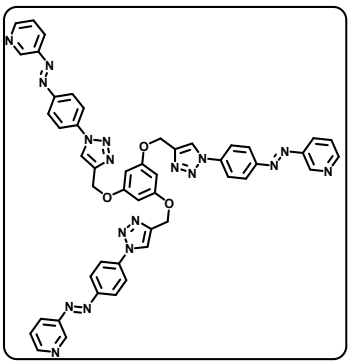
three times with H_2O and acetone. The yellow solid product was further purified by column chromatography using DCM:MeOH (95:5) as an eluent. After removing the solvent through rotary evaporator, the final product was dried under vacuum to yield the desired product.



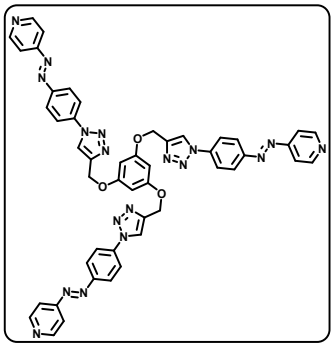
4,4'-(((5-((2-(4-((*E*)-phenyldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1-(4-((*E*)-phenyldiazenyl)phenyl)-1*H*-1,2,3-triazole) (**T1**): Yellow solid, mp= 250-253 °C, 70% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 9.10 (s, 3H), 8.17 (d, J = 8.8 Hz, 6H), 8.09 (d, J = 8.8 Hz, 6H), 7.94-7.92 (m, 6H), 7.62-7.60 (m, 9H), 6.49 (s, 3H), 5.28 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 159.9, 151.9, 151.3, 144.1, 138.2, 132.0, 129.6, 124.2, 123.0, 122.8, 120.9, 94.9, 52.0; FT-IR (ATR): 2923, 2852, 1597, 1502, 1384, 1138, 863, 617 cm^{-1}; HRMS (MALDI): *m/z* calcd. for $C_{51}H_{39}N_{15}O_3$ Na[M+Na]$^+$: 932.3258; found : 932.3243.



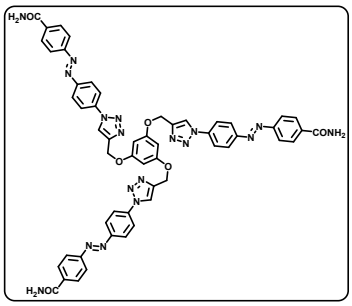
4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-(4-hydroxyphenyl)diazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))diphenol (**T2**): Orange solid, mp= 260-262°C, 80 %yield. ^{1}H NMR (400 MHz, DMSO-d_6):δ (ppm) 10.42 (s, 3H), 9.08 (s, 3H), 8.12 (d, J = 8.4 Hz, 6H), 8.00 (d, J = 8.3 Hz, 6H), 7.84 (d, J = 8.3 Hz, 6H), 6.96 (d, J = 8.5, 6H), 6.49 (s, 3H), 5.27 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 161.4, 159.9, 151.6, 145.2, 144.0, 137.4, 125.2, 123.6, 122.9, 120.9, 116.1, 94.9, 61.1; FT-IR (ATR): 3424, 2922, 2856, 1596, 1508,1386, 1150, 842, 617 cm^{-1}; HRMS (MALDI): *m/z* calcd. for $C_{51}H_{39}N_{15}O_6$ Na[M+Na]$^+$: 980.3106; found : 980.3137.



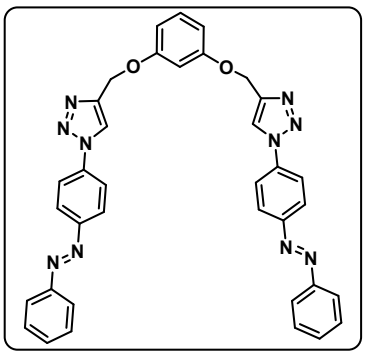
4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-pyridin-4-yldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dipyridine (**T3**): Orange solid, mp= 254-255°C, 70 %yield.^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm)9.13 (s, 3H), 8.23-8.16 (m, 14H), 7.93 (br, 10H), 6.49 (s, 3H), 5.28 (s, 6H); FT-IR (ATR): 2922, 2851, 1600, 1583, 1509, 1194, 849, 705 cm^{-1};HRMS (ESI): *m/z* calcd. for $C_{48}H_{36}N_{18}O_3$ [M+Na]$^+$: 935.3116; found : 935.4329.



3,3'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-pyridin-3-yldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dipyridine (**T4**): Orange solid, mp= 258-259°C, 75 %yield.^{1}H NMR (400 MHz, DMSO-d_6):δ (ppm) 9.12 (s, 3H), 8.22-8.11 (m, 21H), 7.67 (s, 3H), 6.49 (s, 3H), 5.28 (s, 6H); FT-IR (ATR): 2921, 2851, 1600, 1583, 1509, 1194, 848, 704 cm^{-1};HRMS (ESI): *m/z* calcd. for $C_{48}H_{36}N_{18}O_3$ $[M+Na]^+$: 935.3116; found : 935.4329.



4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-(4-carbamoylphenyl)diazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dibenzamide (**T5**): Orange solid, mp= 278-280°C, 70% yield.^{1}HNMR (400 MHz, DMSO-d_6): δ (ppm)9.56 (s, 6H), 9.09 (s, 3H), 8.21-8.01 (dd, J = 61.8, 9.7 Hz,24H), 6.12 (s, 3H), 5.21 (s, 6H);^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 167.6, 153.7, 149.5, 143.5, 136.8, 129.3, 129.2, 125.1, 124.8, 123.0, 122.7, 121.4, 120.6, 31.7;FT-IR (ATR): 3451, 3185, 2923, 1658, 1596, 1410, 1302, 1194, 848, 704 cm^{-1};HRMS (ESI): *m/z* calcd. for $C_{54}H_{42}N_{18}O_6$ $[M+Na]^+$: 1061.3433; found : 1061.4735.

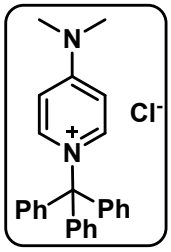


1,3-bis((1-(4-((*E*)-phenyldiazenyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzene (**B1**): Orange solid, 95% yield.^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 9.11 (s, 2H), 8.19 (d, J = 8.9 Hz, 4H), 8.11 (d, J = 8.8 Hz, 1H), 7.95-7.93 (m, 4H), 7.65-7.62 (m, 6H), 7.26 (t, 1H), 6.84 (s, 1H), 6.74-6.71 (dd, , J = 8.2, 2.12 Hz), 5.28 (s, 4H) ; ^{13}C NMR (100 MHz, DMSO-d_6): δ (ppm) 159.7, 152.3, 151.8, 150.4, 144.7, 138.7, 136.3, 130.0,124.6, 123.5, 123.2, 121.4, 108.0, 61.5, 61.49; FT-IR (ATR): 2923, 1675, 1585, 1483, 1362, 1135, 1019 cm^{-1}; HRMS (ESI): *m/z* calcd. for $C_{36}H_{28}N_{10}O_2[M+H]^+$: 633.2475; found : 633.2454.

Synthesis of DMAP-TrCl adduct (A1):[8]

DMAP**14**(1.0 equiv.)andtritylchloride**15**(1.1 equiv.)weremixed in a flame dried Schlenk flask. Dichloromethane(40mL)was dropwise added over 30 minutes. The resulting solution was stirred for3h at rt.Ethylacetate(200mL)wasthen added dropwise over 1h. The inhomogeneous reaction mixturewaskept in a refrigerator for 10 minutes to obtain maximum precipitation of the salt. The products were filtered off,washed with dry ethylacetate(30mL)and dried at high vacuum to obtain the desired product trityl-DAMP-salt

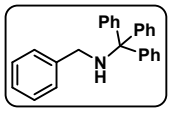
as a white semi-crystallinesolid (It was found to be a DCM-adduct with 0.75 eq. of dichloromethane).



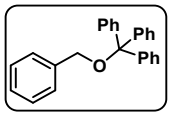
4-(Dimethylamino)-1-tritylpyridin-1-ium chloride (**A1**): White solid, mp= 116-118 °C, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.91-7.87 (m, 2H), 7.40-7.35 (m, 9H), 7.21-7.18 (m, 2H), 7.14-7.10 (m, 6H), 3.38 (s, 6H)

General procedure for the reactions:[8]

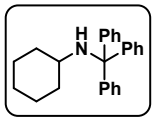
DMAP-TrCl·0.75CH_2Cl_2adduct **A1** (1.0equiv.) and catalyst **T1-5** or **B1**(0.05 equiv.) were suspended in DCM (0.5mL) in a 10mL screw cap vial. The corresponding amine or alcohol (**R1-4**)(2.0equiv.) was added. The resulting mixture was stirred for 9 h at rt. Purification of the crude mixture by column chromatography on deactivated silica providedthe desired *N*- or *O*-tritylated product. (The catalyst may be used either as a native solid or photoswitched with 365 nm irradiation after dissolved in any of the solvents; For uncatalyzed reactions, the reaction procedures were the same except the addition of the catalyst.)



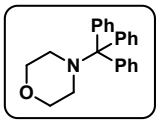
N-Benzyl-1,1,1-triphenylmethanamine (**P1**): White solid, mp= 103-106 °C, 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.59-7.57 (d, *J*= 8 Hz, 6H), 7.43-7.20 (m, 14H), 3.35 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 146.1, 141.0, 128.4, 128.2, 127.8, 127.6, 126.5, 126.2, 70.6, 47.4.



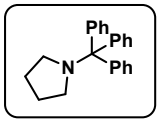
((Benzyloxy)methanetriyl)tribenzene (**P2**): White solid, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.55-7.53 (d, *J*= 7.5 Hz, 6H), 7.43-7.24 (m, 14H), 4.20 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 144.2, 139.3, 128.9, 128.4, 128.0, 127.21, 127.15, 127.1, 87.1, 66.0.



N-Tritylcyclohexanamine (**P3**): White solid, mp= 126-128 °C, 55% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.61-7.59 (m, 6H), 7.30-7.26 (m, 6H), 7.21-7.17 (m, 3H), 2.32-2.26 (m, 1H), 1.60 (s, 1H), 1.52-1.42 (m, 4H), 1.24-1.21(m, 2H), 1.0-0.85 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 147.6, 128.9, 127.8, 126.2,71.4, 52.2, 35.9, 26.1, 25.8.



N-Tritylmorpholine(**P4**): White solid, mp= 185-187 °C, 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.40 (brs, 6H), 7.33-7.29(m, 6H), 7.20-7.17 (m, 3H), 3.73 (s, 4H), 2.67 (brs, 1H), 1.49-1.23 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 129.0, 128.9, 127.7, 126.1,76.5, 66.6, 48.4.



N-Tritylpyrrolidine(**P5**): White solid, mp= 124-126 °C, 54% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm) 7.41-7.39 (m, 6H), 7.31-7.27 (m, 6H), 7.20-7.15 (m, 3H), 2.21 (s, 4H), 1.57 (s, 4H); ^{13}C NMR (100 MHz, DMSO-d_6): δ(ppm) 142.5, 128.9, 127.4, 126.0,73.9, 45.8, 21.9.

S3. Photoswitching studies of the catalysts T1-5 and B1

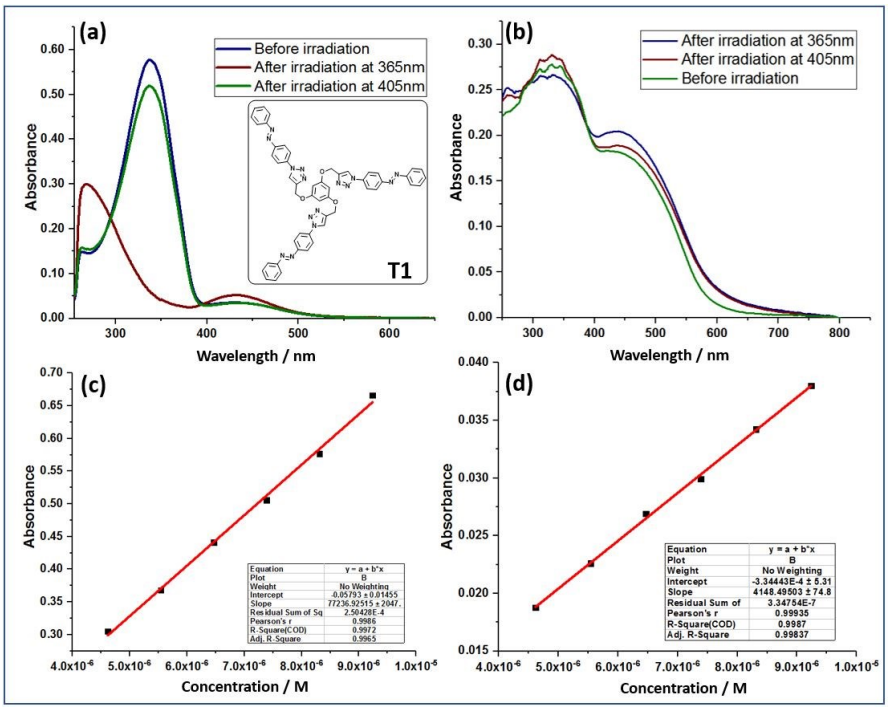


Fig. S1. UV-Vis spectroscopic data of **T1**: (a) Photoswitching studies performed in DMSO (9 μM); (b) Photoswitching studies performed in KBr medium; Estimation of molar absorption coefficient for (c) π–π* absorption maxima and (d) n–π* absorption maxima.

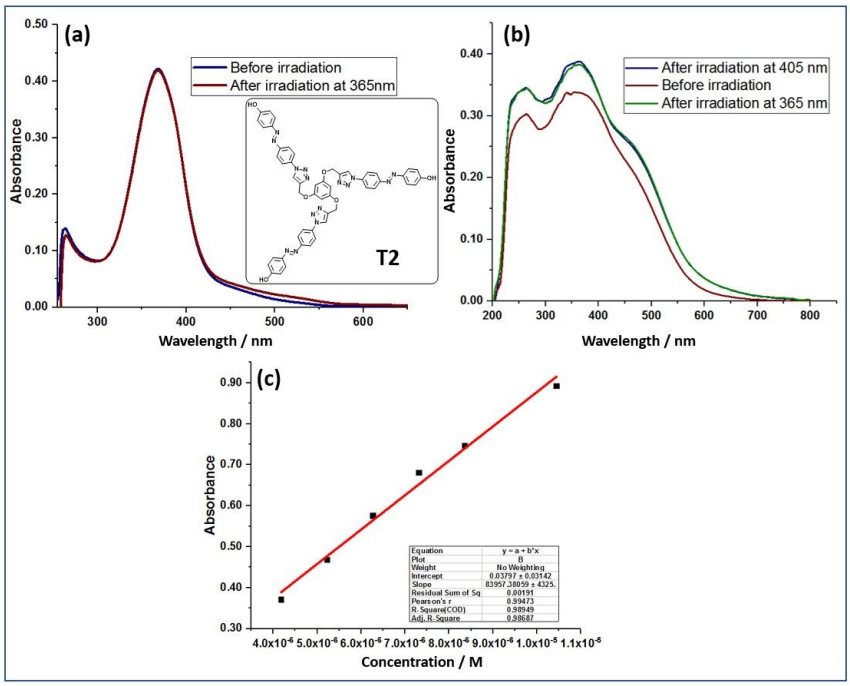


Fig. S2. UV-Vis spectroscopic data of **T2**: (a) Photoswitching studies performed in DMSO (10 μM); (b) Photoswitching studies performed in KBr medium; Estimation of molar absorption coefficient for (c) π–π* absorption maxima and (d) n–π* absorption maxima.

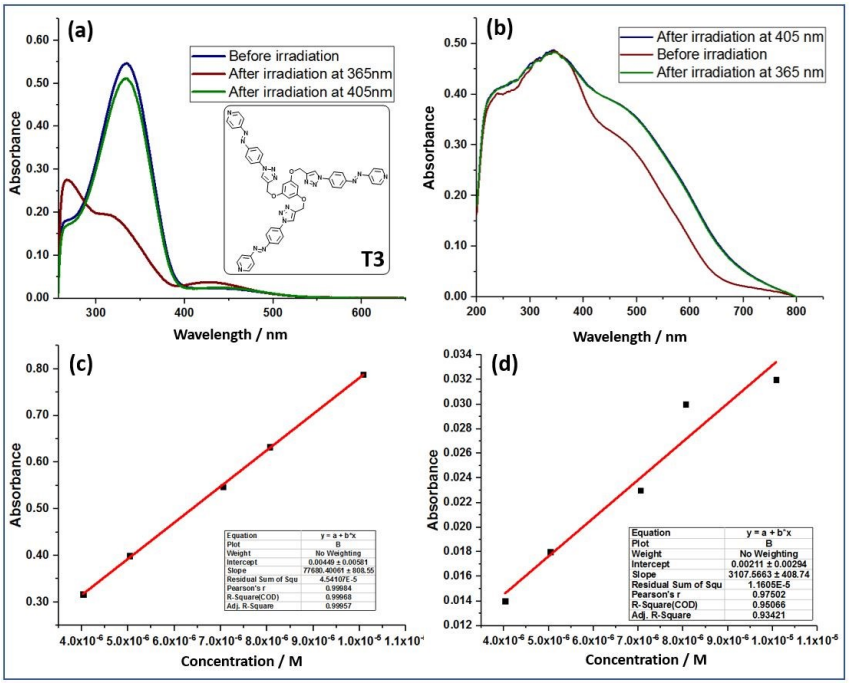


Fig. S3. UV-Vis spectroscopic data of **T3**: (a) Photoswitching studies performed in DMSO (10 μM); (b) Photoswitching studies performed in KBr medium; Estimation of molar absorption coefficient for (c) π–π* absorption maxima and (d) n–π* absorption maxima.

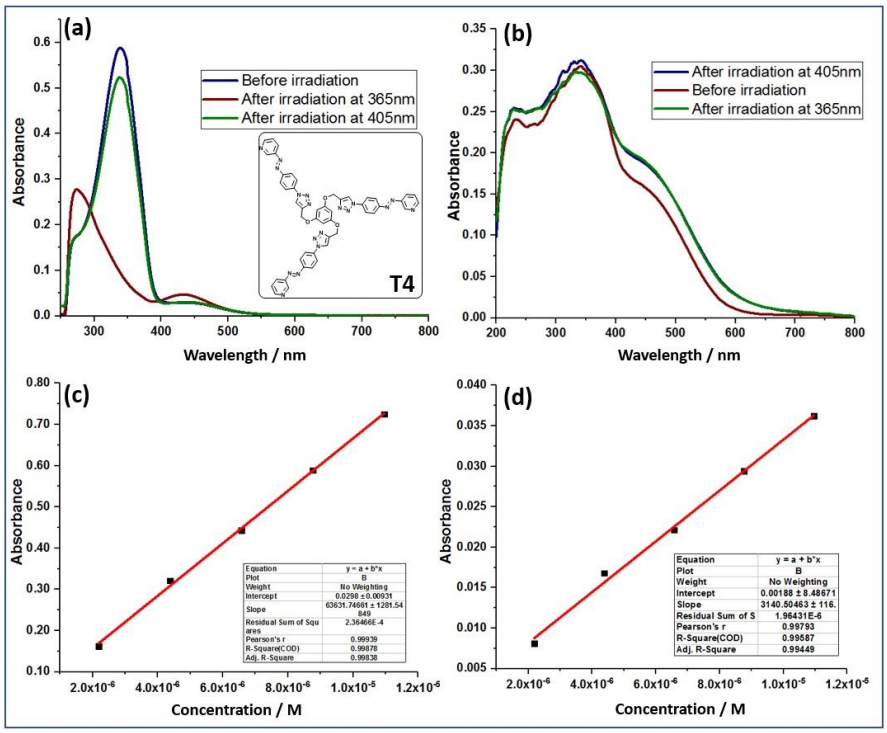


Fig. S4. UV-Vis spectroscopic data of **T4**: (a) Photoswitching studies performed in DMSO (11 μM); (b) Photoswitching studies performed in KBr medium; Estimation of molar absorption coefficient for (c) π–π* absorption maxima and (d) n–π* absorption maxima.

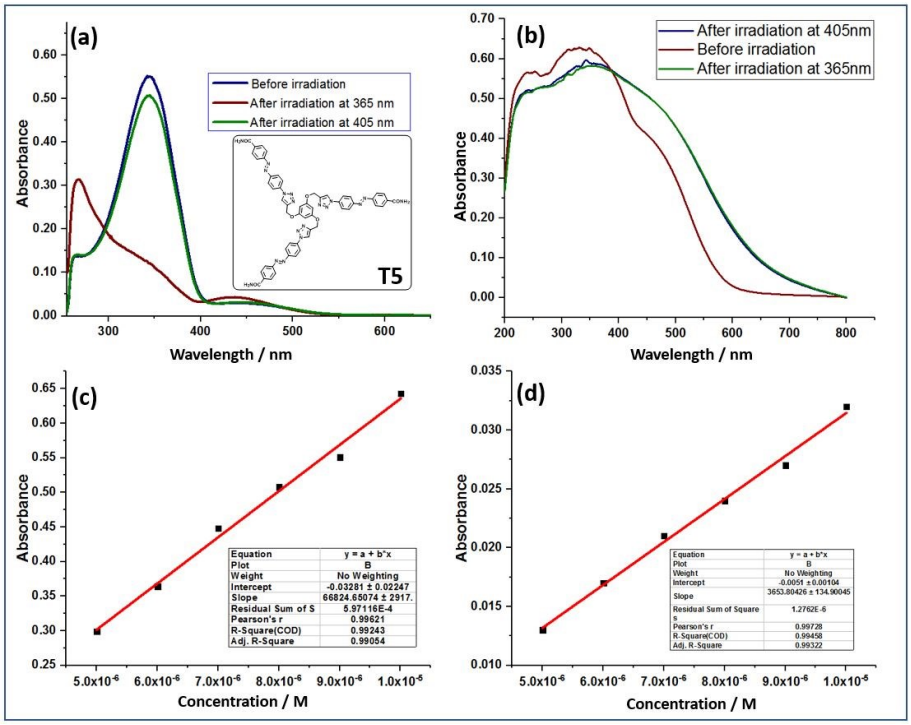


Fig. S5. UV-Vis spectroscopic data of **T5**: (a) Photoswitching studies performed in DMSO (10 μM); (b) Photoswitching studies performed in KBr medium; Estimation of molar absorption coefficient for (c) π–π* absorption maxima and (d) n–π* absorption maxima.

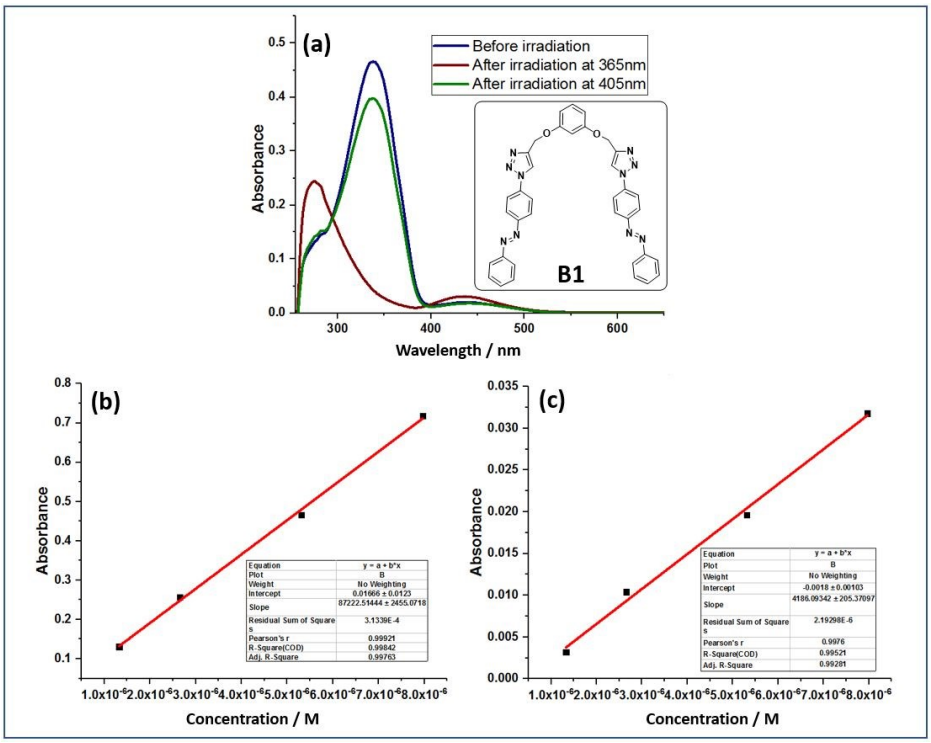


Fig. S6. UV-Vis spectroscopic data of **B1**: (a) Photoswitching studies performed in DMSO (13 μM); Estimation of molar absorption coefficient for (b) π–π* absorption maxima and (c) n–π* absorption maxima.

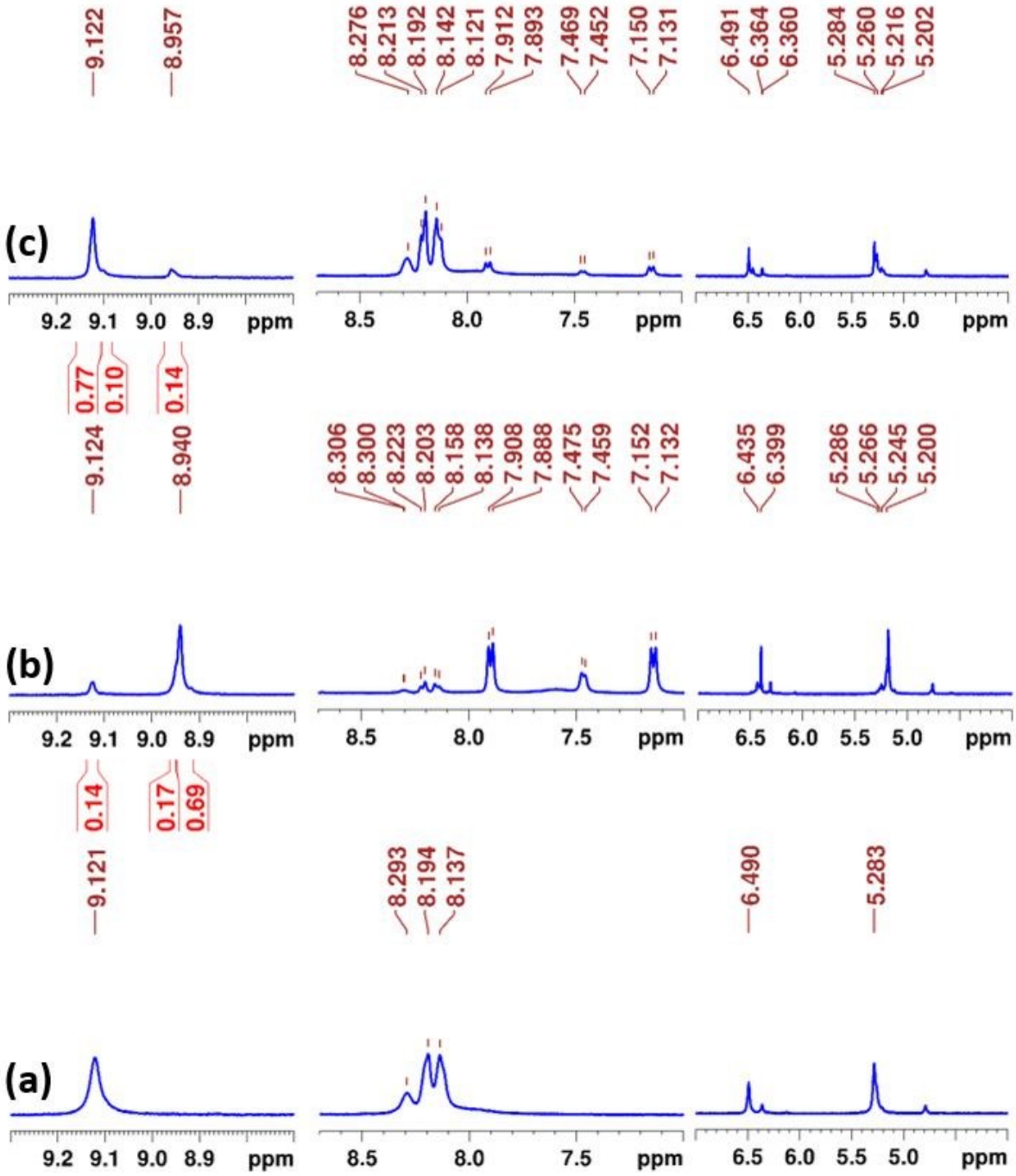


Fig. S7. Photoswitching in catalyst **T4**. ^{1}H-NMR spectral data (DMSO-d_6, 11 mM): (a) Before irradiation; (b) After irradiation at 365 nm; (c) After irradiation at 405 nm. (The PSS compositions have been estimated using the normalized integral values corresponding to triazole-CH signals).

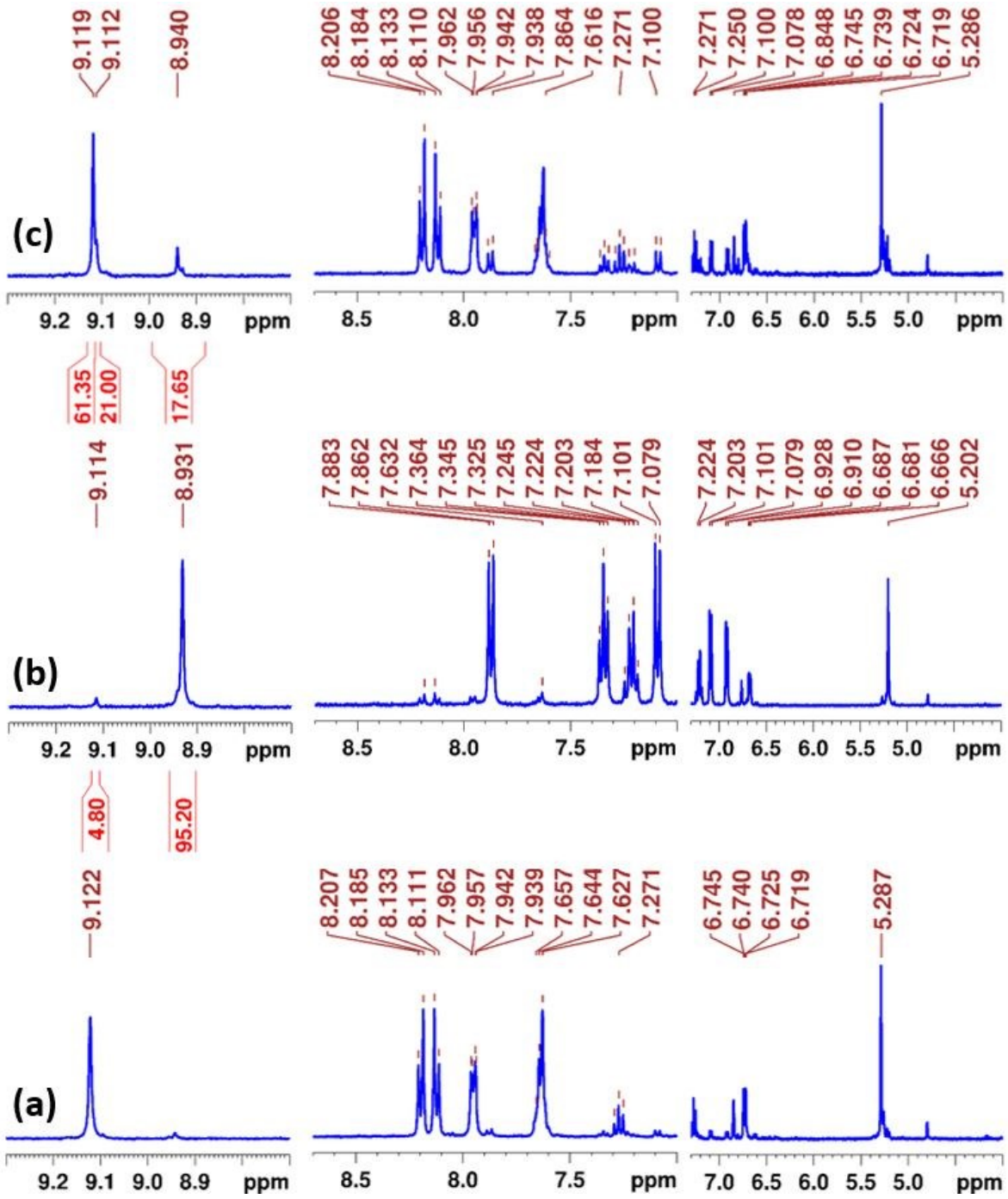


Fig. S8. Photoswitching in catalyst **B1**. ^{1}H-NMR spectral data (DMSO-d_6, 13 mM): (a) Before irradiation; (b) After irradiation at 365 nm; (c) After irradiation at 405 nm. (The PSS compositions have been estimated using the normalized integral values corresponding to triazole-CH signals).

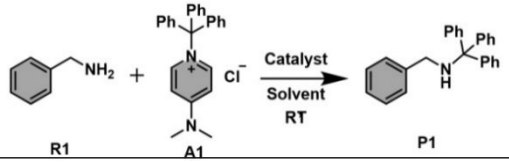
Table S1. Electronic spectroscopic data and analysis of photoswitching properties of the catalysts **T1-5** and **B1** using UV-Vis and NMR spectroscopic data:

S. No.	Catalyst	UV-Vis spectroscopic data[a]				^{1}H-NMR spectroscopic data[b]				
		Native isomer		After 365 nm irradiation		PSS composition				C [mM]
		π-π* (λ_{max}/ε)	n–π* (λ_{max}/ε)	π-π* (λ_{max})	n–π* (λ_{max})	%*EEE*	%*EEZ*	%*EZZ*	%*ZZZ*	
1.	**T1**	338 (77237±2047)	442 (4148±75)	269	432	0 **84**	0 **0**	16 **14**	84 **<2**	11
2.	**T2**	368 (83957±4325)	-	-	-	-	-	-	-	-
3.	**T3**	335 (77680±808)	441 (3107±408)	267	431	14 **77**	- **10**	17 **13**	69 -	11
4.	**T4**	339 (63632±1281)	440 (3140±116)	274	439	-	-	-	-	-
5.	**T5**	342 (66825±2917)	441 (3654±135)	268	437	-	-	-	-	-
6	**B1**	338 (87222±2455)	448 (4186±205)	275	435	5 **61**	- **21**	- **18**	95 -	16

[a]The λ_{max} and ε values are expressed in nm and L.mol^{-1}.cm^{-1}, respectively. [b]The PSS composition for forward (at 365 nm, normal font) and reverse isomerization (at 405 nm, bold font) were estimated using the normalized integral values of triazole C-H signals from the ^{1}H-NMR spectral data.

S4. Reaction condition optimization

Table S2. Optimization of reaction conditions*:



Entry	Catalyst	Catalyst loading (mol%)	Solvent	Time (hrs)	Yield # (%)
1	***EEE*-T1**	10	DCM	9	85
2	***EEE*-T1**	5	DCM	9	82
3	**none**	none	DCM	9	52
4	***EEE*-T1**	10	DMSO	9	80
5	***EEE*-T1**	5	DMSO	9	80
6	**none**	none	DMSO	9	45
7	***EEE*-T1**	10	THF**	9	20
8	***EEE*-T1**	5	THF**	9	20
9	**none**	none	THF**	9	0
10	***EEE*-T1**	3	DCM	9	72
11	***EEE*-T1**	2	DCM	9	68
12	***EEE*-T1**	5	DCM	7	72
13	***EEE*-T2**	5	DCM	9	70
14	***EEE*-T2**	5	DMSO	9	40
15	***EEE*-T3**	5	DMSO	9	60
16	***EEE*-T4**	5	DMSO	9	68
17	***EEE*-T5**	5	DMSO	9	34
18	***ZZZ*-T1[a]**	5	DMSO	9	78
19	***ZZZ*-T1[b]**	5	DMSO	9	72
20	***ZZZ*-T1[c]**	5	DMSO	9	68
21	***ZZZ*-T1[d]**	5	DMSO	9	55
22	***ZZZ*-T1[e]**	5	DMSO	9	38
23	***ZZZ*-T1[f]**	5	DCM	9	38

*Conditions: **R1** (22.9 μL, 0.21 mM), **A1** (50 mg, 0.10 mM), 0.5 mL solvent; #Isolated yields; **In THF, the catalyst was insoluble; The catalyst was irradiated at 365 nm [a]in DMSO for 1 min; [b]in DMSO for 3 min; [c]in DMSO for 5 min; [d]in DMSO for 30 min; [e]in DMSO for 40 min; [f]in DCM for 40 min; Irradiation was done in the presence of DMAP-TrCl salt in each case.

Control experiments:

(a) In order to verify the influence of column condition or work up procedure in controlling the yields, we have also performed the purification using alumina column and also a work up using a base wash, before evaporation of solvent and column purification. However, we did not observe any changes in the yields with respect to the photoswitching of the catalysts.

(b) Under higher catalytic loading, we observed solubility issues and so the understanding the effects of photoswitching was unsuccessful. Interestingly, the parent catalyst was showing a partial photoswitching in solid state, however to a limited extent.

(c) In many solvents, the presence of moisture influences the reaction rates. Upon using dry solvents, the yields were found to be lower than the indicated values. For instance, when dry DMSO was used as a solvent, the yields were found to be 15%, 42% and 10% for the uncatalyzed, ***EEE*-T1** and ***ZZZ*-T1** catalysed reactions, respectively. As reported by Hirata et al., we also observed moderate yields in certain solvents even without the catalyst.[9] However, under identical conditions, the native and photoswitched catalyst showed remarkable difference in the yields, indicating rate changes by the catalyst.

S5. Forward isomerization kinetics experiments (NMR and UV-Vis spectroscopic studies)

Photoswitchable catalyst **T1** upon irradiation using 365 nm light gives a mixture of different photoisomers, namely ***ZZZ***-, ***ZZE***-, and ***ZEE***- along with the residual native isomer ***EEE*-T1** have been formed. The Forward isomerisation kinetics have been followed using a 400 MHz NMR and UV-Vis spectrophotometer at 298 K. For following the kinetics, the sample (as a solution either in a quartz NMR tube (for NMR experiments) or in a quartz cuvette (for UV-Vis spectroscopic experiments)) has been kept at a distance of 4 cm from the light source. The observed rate of forward isomerization kinetics experiments performed by using NMR and UV-Vis spectroscopy are found to be 4.43 x 10^{-2} and 9.14 x 10^{-2}, respectively (Fig. S10). The corresponding data for the estimation of rate constant through NMR spectroscopy and changes in the composition of ***ZZZ*-T1** over a period of 60 minutes have been shown as stacking plot in **Fig. S11**.

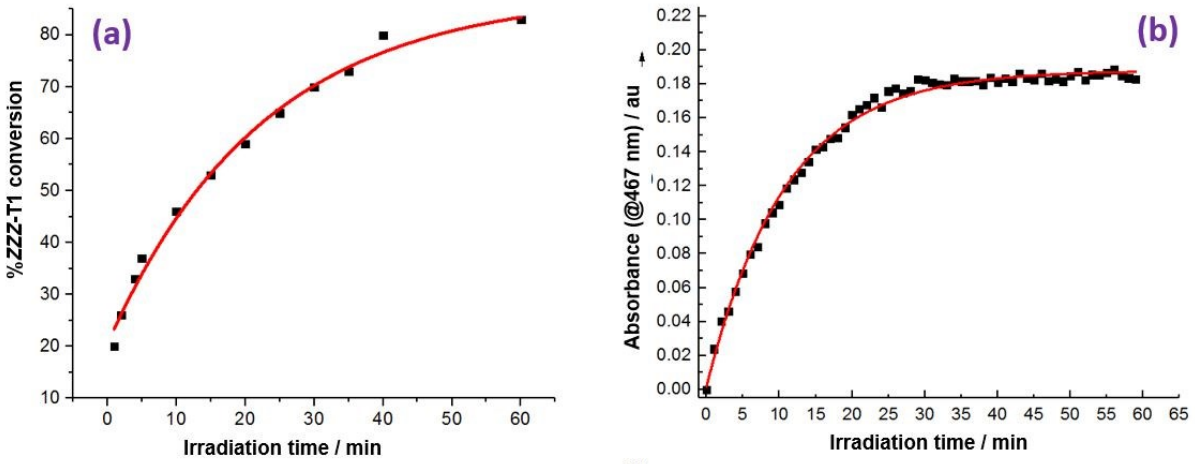


Fig. S9. Forward isomerization rate plots for the conversion of ***EEE*-T1** to ***ZZZ*-T1** up to the attainment of PSS using (a) ^{1}H-NMR (Solvent: DMSO-d_6; 11 mM; Forward isomerization rate constant, k_f = 4.43 x 10^{-2} ± 5.5 x 10^{-3} min^{-1}) and (b) UV-Vis spectroscopy (Solvent: DMSO; 11 mM; Forward isomerization rate constant, k_f = 9.14 x 10^{-2} ± 2.0 x 10^{-3} min^{-1}) (Both samples were irradiated with 365 nm LED light source of intensity 7 mW at a fixed distance of 4 cm).

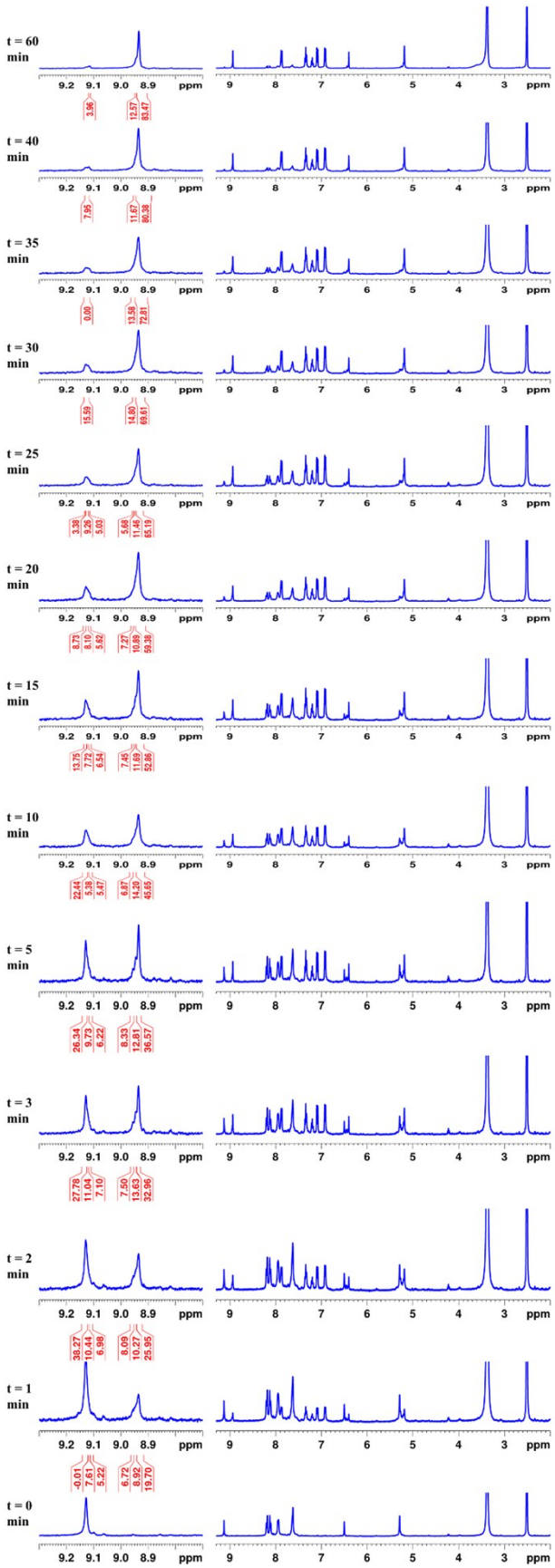


Fig. S10. Photoswitching in catalyst **T1**. ^{1}H-NMR spectral data (DMSO-d_6, 11 mM) for the estimation of forward isomerisation rate constant at different irradiation times (365 nm LED light source of intensity 7 mW at a fixed distance of 4 cm was used for irradiation)

S6. Evaluation of time profiles for the reactions with the catalyst (*EEE*-T1 and *ZZZ*-T1)

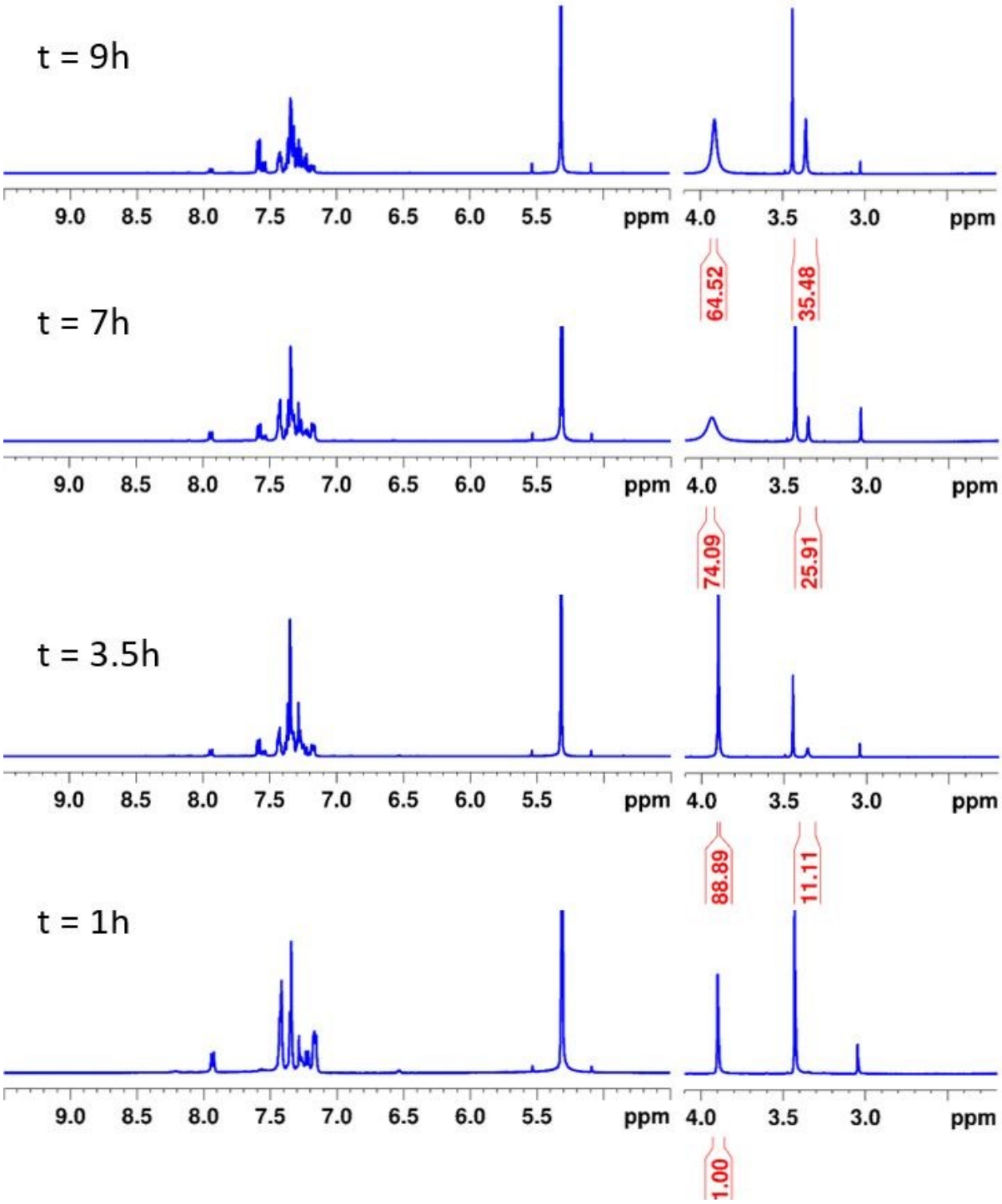


Fig. S11a. ^{1}H-NMR experiment depicting the conversion of tritylated benzylamine using **(*ZZZ*)-T1** as a catalyst. (All the NMR spectra have been recorded in $CDCl_3$ for the crude reaction mixture collected at different intervals of time as indicated in the spectra; The normalized integral values corresponding to CH_2 protons of the reactant and the product have been used for the estimation of conversion. The reaction was conducted with the following conditions: $BzNH_2$ **R1**(22.91 μL, 2.0 eq.), DMAP-TrCl adduct **A1**(50 mg, 1.0 eq.), **(*ZZZ*)-T1** (5 mol%) in 0.5 mL DCM).

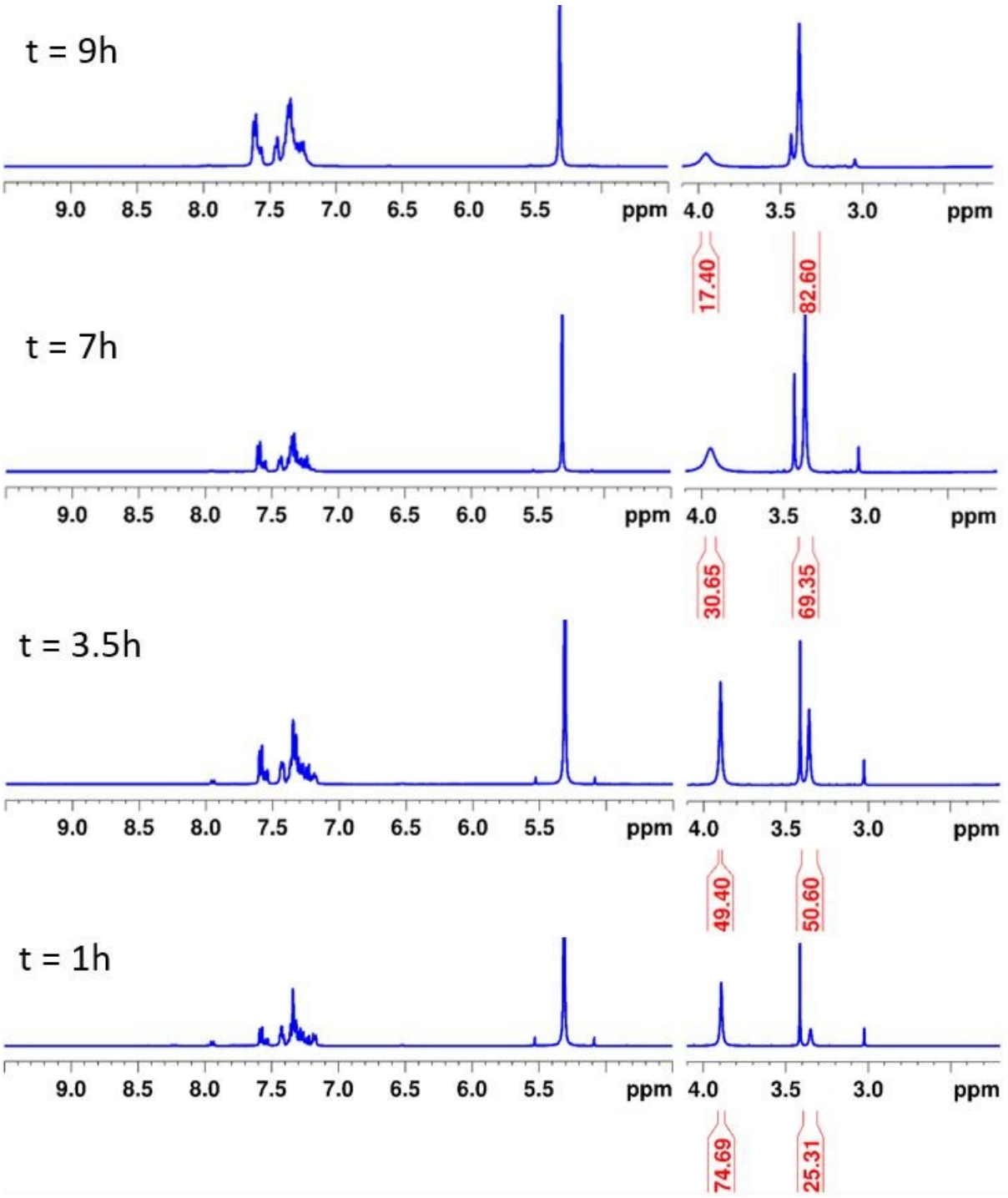


Fig. S11b. ^{1}H-NMR experiment depicting the conversion of tritylated benzylamine using **(*EEE*)-T1** as a catalyst. (All the NMR spectra have been recorded in $CDCl_3$ for the crude reaction mixture collected at different intervals of time as indicated in the spectra; The normalized integral values corresponding to CH_2 protons of the reactant and the product have been used for the estimation of conversion. The reaction was conducted with the following conditions: $BzNH_2$ **R1** (22.91 μL, 2.0 eq.), DMAP-TrCl adduct **A1** (50 mg, 1.0 eq.), **(*EEE*)-T1** (5 mol%) in 0.5 mL DCM).

S7. Reverse thermal isomerization kinetics data

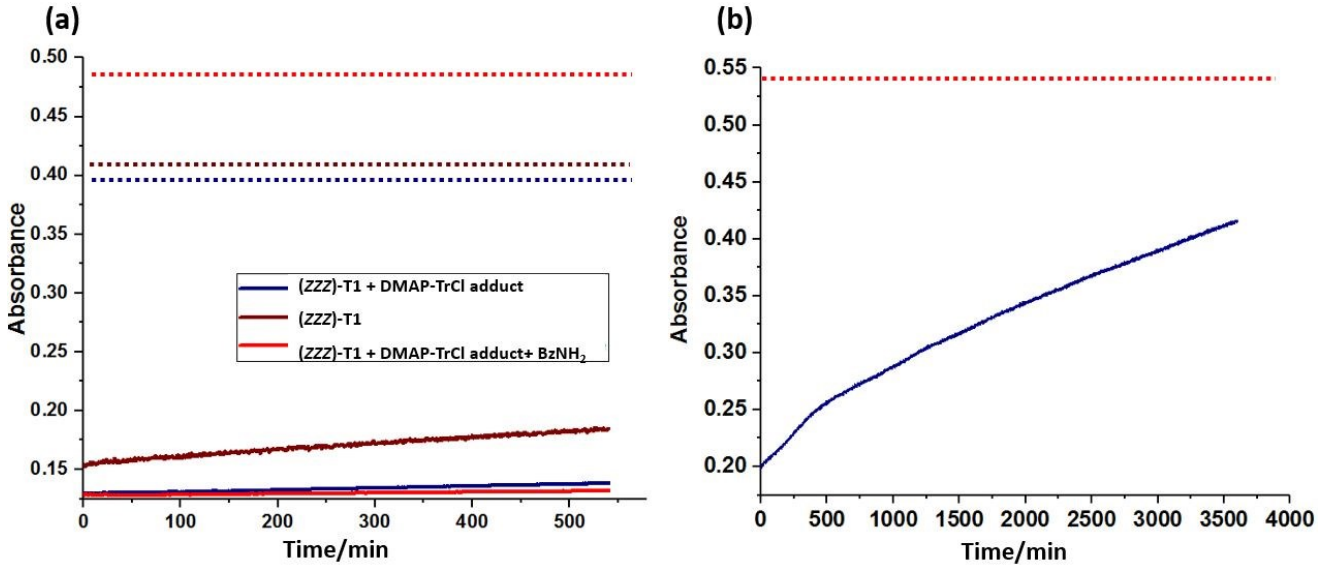


Fig. S12. Kinetics profiles depicting the thermal stability of photoisomerized state (*ZZZ*) of the catalyst **T1** (a) up to 9 h (the optimized reaction time) using UV-Vis spectroscopy in DMSO; The dotted lines indicate the absorption maxima due to the ***EEE*-T1** under the respective conditions (prior to irradiation at 365 nm); (b) up to 60 h (The dotted lines indicate the absorption maxima due to the ***EEE*-T1**).

The stability of ***ZZZ*-T1**was measured by estimating the % of the catalyst ***ZZZ*-T1** undergoing thermal reverse isomerization after 9 hours using the following expression:

$$\%\ \text{conversion of } ZZZ\text{-isomer} = \frac{A(\pi-\pi*)\ after\ 9h\ -\ A(\pi-\pi*)\ at\ initial\ time}{A(\pi-\pi*)\ before\ irradiation} \times 100$$

$$= \frac{A_{9h}(\pi-\pi*)\ -\ A_0(\pi-\pi*)}{A_\infty(\pi-\pi*)} \times 100$$

Table S3. Kinetic stability of ***ZZZ*-T1**:

S. No.	System	Conditions	% conversion after 9 h
1	***ZZZ*-T1**	DMSO,7 µm, 25±1 °C	<8
2	***ZZZ*-T1** + DMAP-TrCl adduct	DMSO, 1:0.05, 25±1 °C	<2
3	***ZZZ*-T1** + DMAP-TrCl adduct + $BzNH_2$	DMSO, 1:0.05:2, 25±1 °C	<2

S8. HRMS data for the binding of chloride ion with the catalyst T1

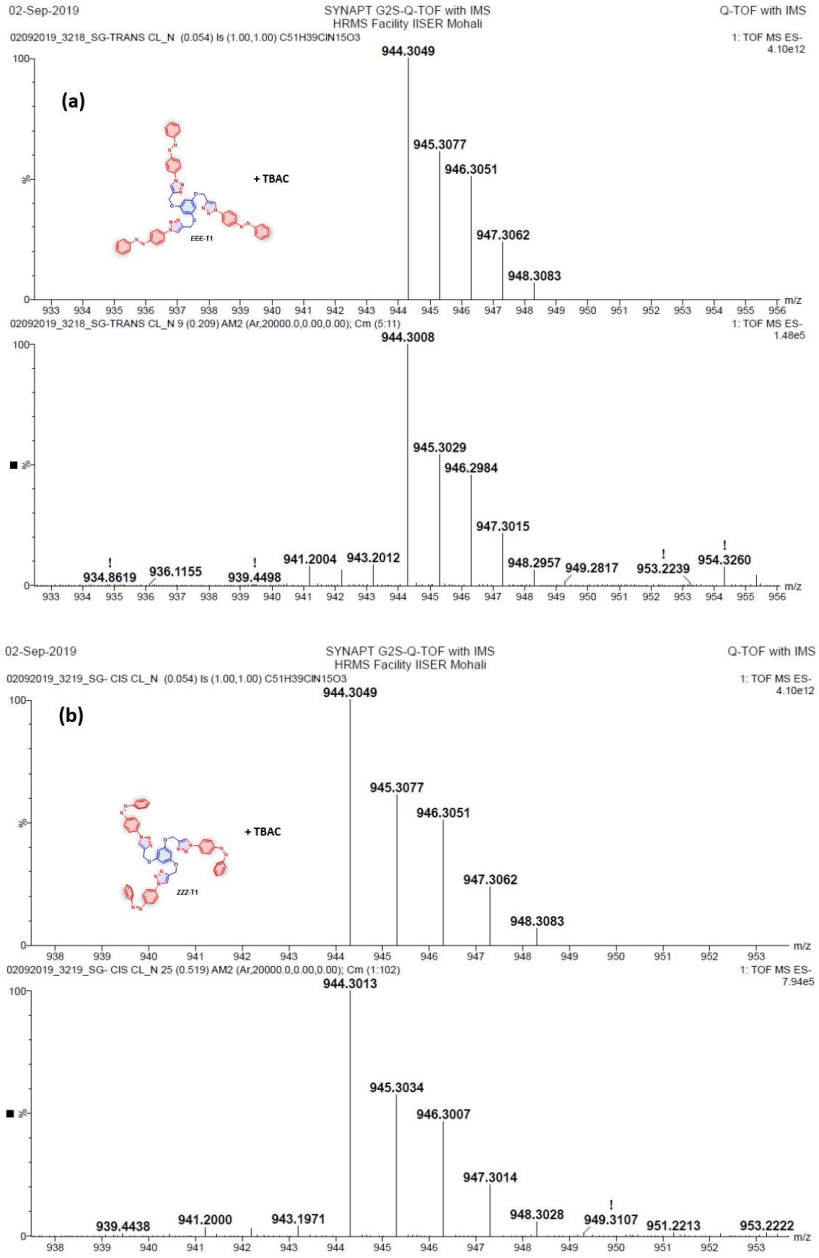


Fig. S13. HRMS data depicting the binding of the catalyst **T1** with chloride ion (as TBAC salt): (a) in native state; (b) after subjecting it to 365 nm irradiation; (HRMS data have been collected in the negative mode using ESI method; Theoretically predicted mass spectral data (top) and experimental data (bottom) are given.)

Table S4. HRMS data of the catalyst **T1** binding with various anions:

S. No.	Guest	Host	Exact mass	Observed mass	Description	Mass error (ppm)
1.	TBAC	***EEE*-T1**	944.3049 946.3051	944.3008 946.2984	$[M + {}^{35}Cl^-]$ $[M + {}^{37}Cl^-]$	4 5.3
2.	TBAC	***ZZZ*-T1**	944.3049 946.3051	944.3013 946.3007	$[M + {}^{35}Cl^-]$ $[M + {}^{37}Cl^-]$	4 4.5

S9. NMR titration experiments

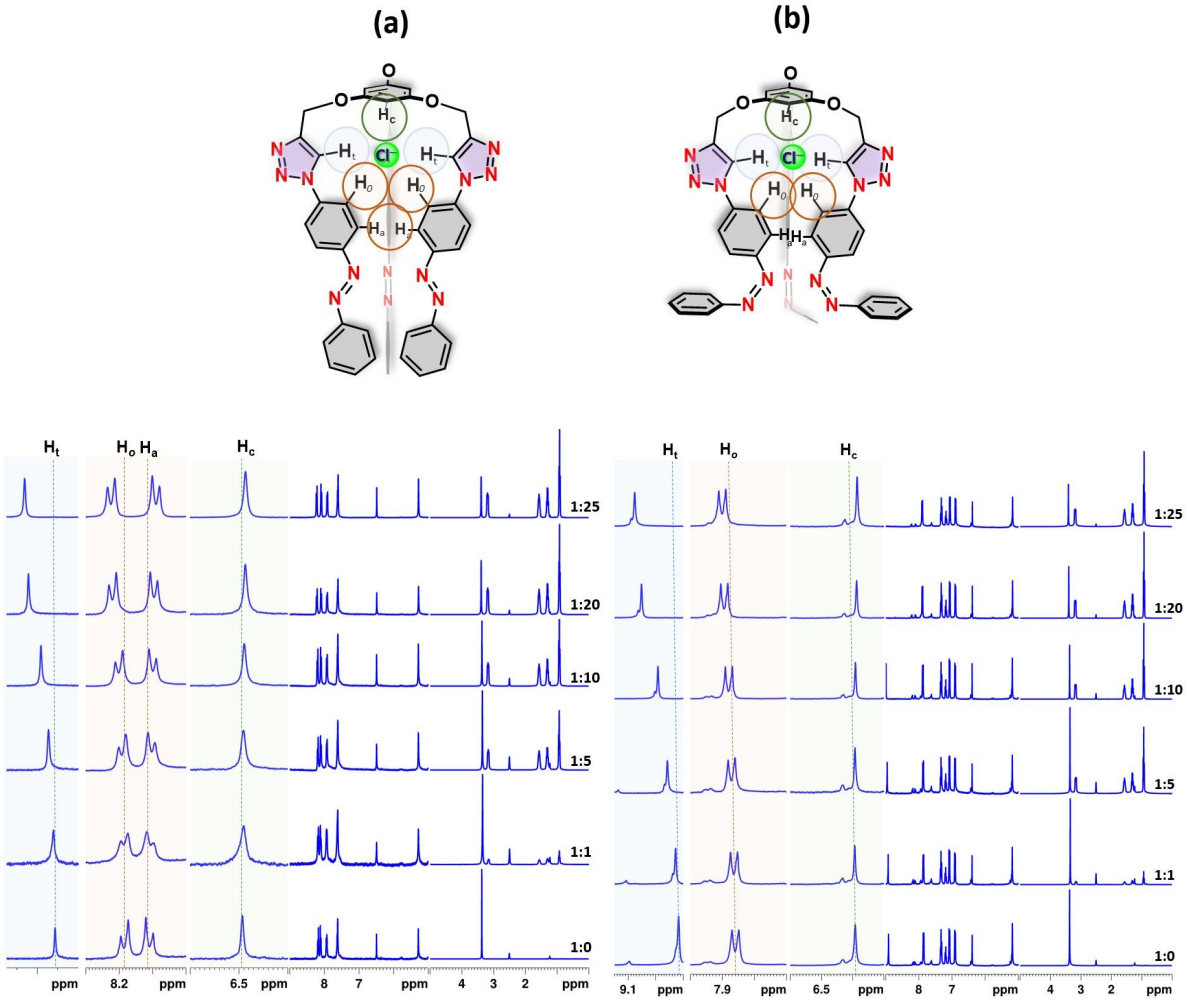


Fig. S14. ^{1}H-NMR experiment depicting the shifts in the catalyst **T1** upon titration with TBAC with a stoichiometric ratios (**T1**:TBAC): (a) 1:0; (b) 1:1; (c) 1:5; (d) 1:10; (e) 1:20 and (f) 1:25. (left: for the native state of ***EEE*-T1** and right: after photoswitching at 365 nm) [Concentrations: **T1** – 11 mM] (The protons exhibiting major shifts upon addition of chloride ions are depicted separately. The position of the respective proton signals without chloride ion is indicated through a dotted line. Although methylene protons of the linker part showed upfield shifts, we observed broadness in the signals upon increasing the concentration of chloride ions.)

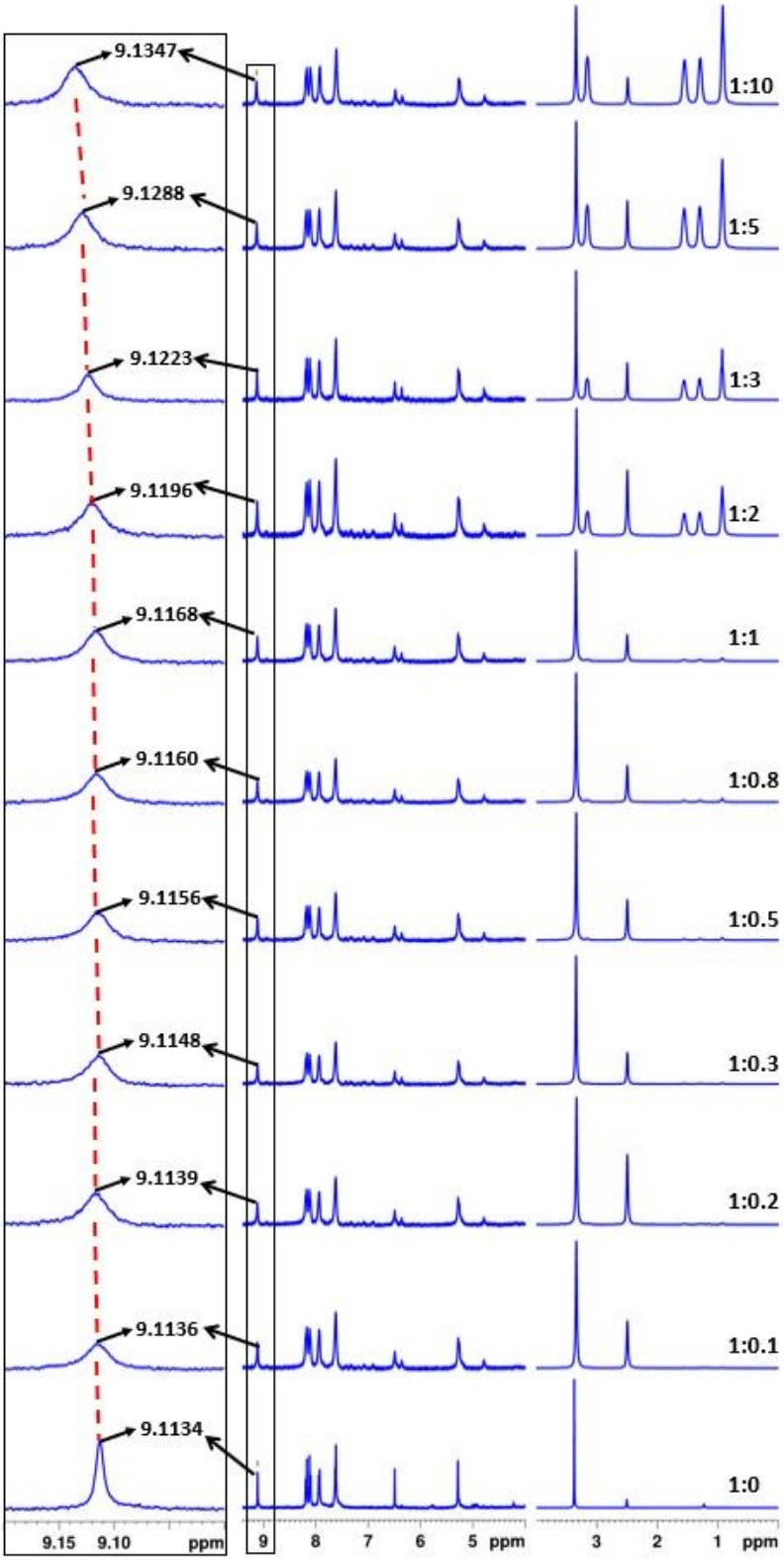


Fig. S15. ^{1}H-NMR experiment depicting the shifts in the catalyst **T1** upon titration with TBAC with stoichiometric ratios (**T1**:TBAC) as follows (bottom to top): 1:0; 1:0.1; 1:0.2; 1:0.3; 1:0.5 1:0.8; 1:1; 1:2; 1:3; 1:5 and 1:10. (for the native state of ***EEE*-T1**) [Concentrations: **T1** – 5.4 mM in DMSO-d_6]

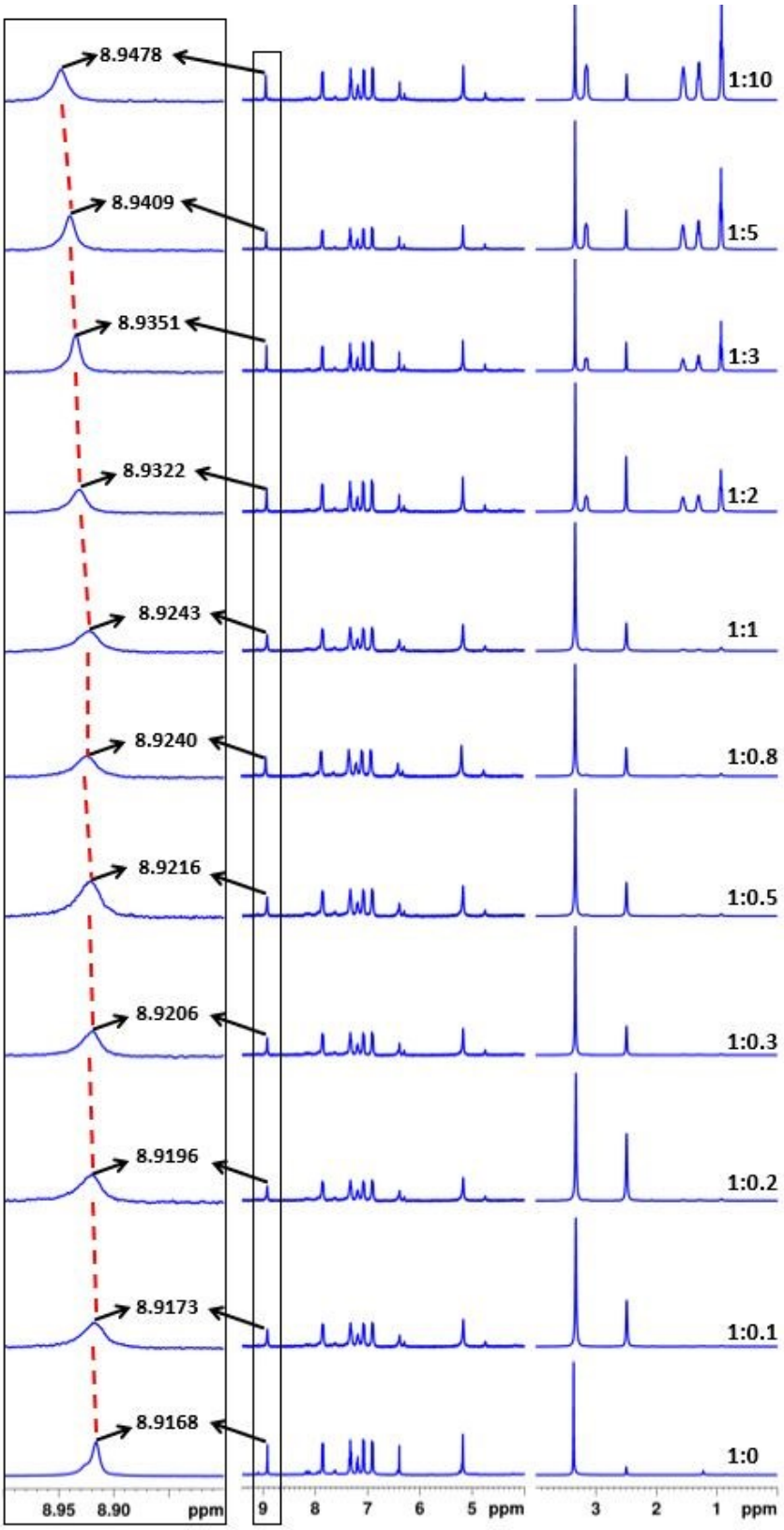


Fig. S16. ^{1}H-NMR experiment depicting the shifts in the catalyst **T1** upon titration with TBAC with stoichiometric ratios (**T1**:TBAC) as follows (bottom to top): 1:0; 1:0.1; 1:0.2; 1:0.3; 1:0.5 1:0.8; 1:1; 1:2; 1:3; 1:5 and 1:10. (after photoswitching at 365 nm) [Concentrations: **T1** – 5.4 mM in DMSO-d_6]

S10. Isothermal Titration Calorimetry (ITC)

Binding affinity of the chloride ions with tripodal triazole linked azoarene **T1** was measured using Isothermal Titration Calorimetry (ITC). This is the gold standard approach for the determination of binding constant (K), and the thermodynamic parameters associated with binding interactions (ΔH, ΔS, ΔG). The experiment was carried out by MicroCal PEAQ-ITC200 (Malvern) at 293.15 K, by titrating the ligand (TBAC) and the substrate (**T1**, Catalyst), wherein the ligand (55.49 mM) was kept in the syringe (Volume = 40 µl) and the substrate (native as well as in photoswitched state) was filled in the cell (Volume = 280 µl) (**T1**, 0.733 mM). Two-µl of the ligand was injected for 4 s through an automated injector into the cell at an interval of 300 s. The contents inside the cell were stirred at 750 rpm to assure proper mixing of the contents. Appropriate blanks experiments were conducted for data analysis. In order to check the biding affinity of the chloride ion with the photoswitched state, the native catalyst is exposed to UV light (λ = 365 nm) for a duration of 30 min, prior to start of the experiment.

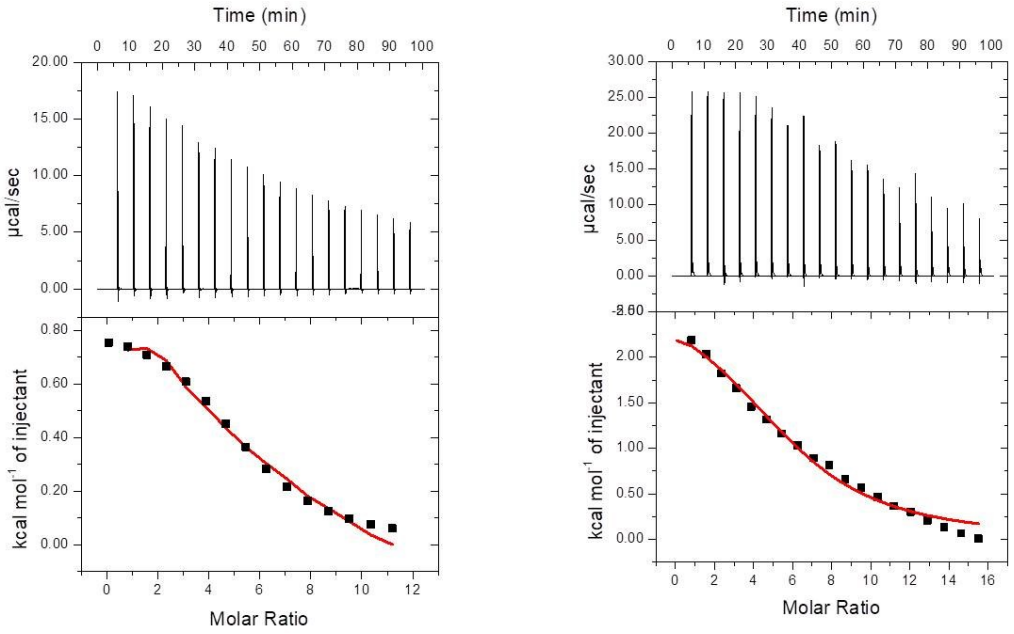


Fig. S17. Estimation of binding constants using isothermal calorimetry: Experimental data and sigmoidal fittings for the binding constant of (a & b) *ZZZ*-T1 with chloride ions (TBAC); (c & d) *EEE*-T1 with chloride ions, respectively. (TBAC: 55.49 mM; *EEE*-T1 and *ZZZ*-T1: 0.733 mM; Addition rate: 2 µL/4 Sec; Temperature: 20 ^{o}C)

S11. Computational data

Geometry optimization have been performed for all the isomeric species of **T1** (*EEE*-, *EEZ*-, *EZZ*- and *ZZZ*-) in their native state, and as complexes with Cl^- ions using density functional theory at B3LYP[11]/6-311G(d,p)[12]level of theory. All the geometries have been optimized to their minima on the potential energy surface and confirmed using frequency calculations. (No imaginary frequencies corresponding to minima). In addition to that, relative energies and Mulliken charges analysis have been performed for all four *EEE*-, *EEZ*-, *EZZ*- and *ZZZ* isomers with the Cl^- ion[8,13] Natural bond orbital (NBO) analysis has been performed to quantify the interaction energies at M06-2X/6-311G(d,p) level of theory.[14] All these calculations were performed using Gaussian09 suite of program.[15]

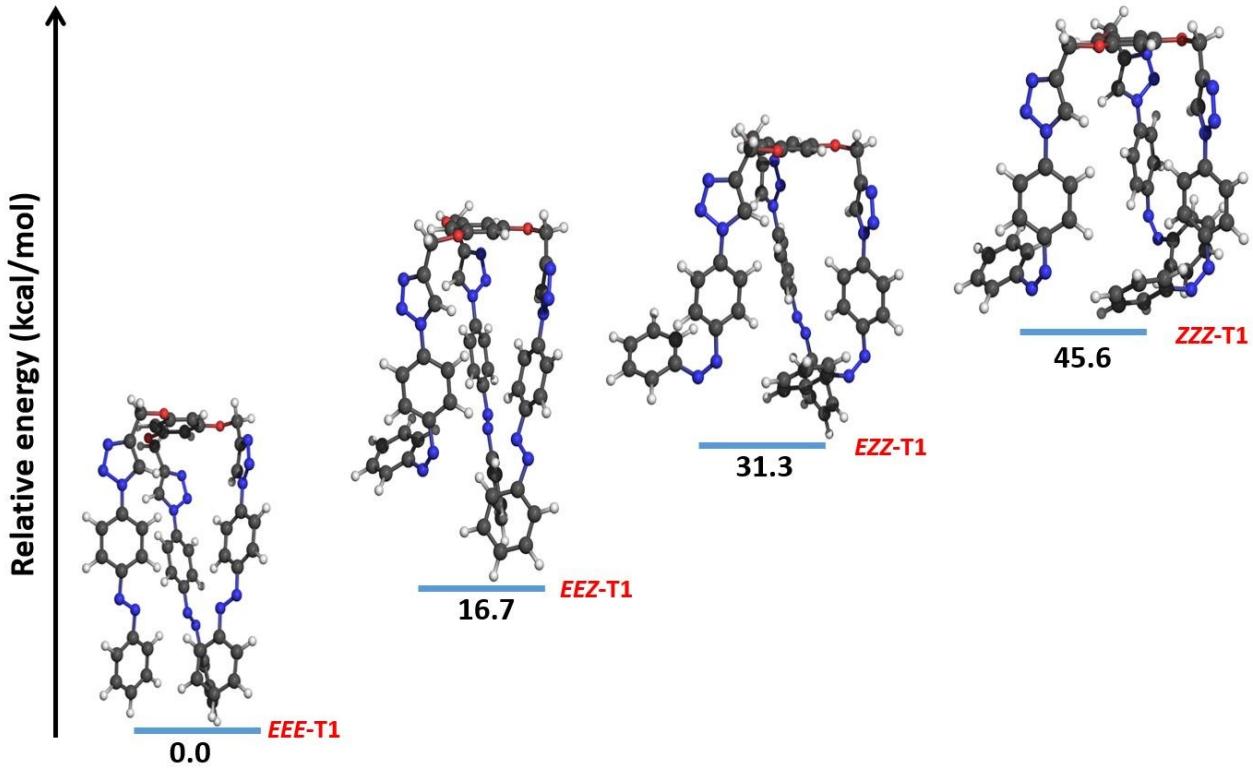


Fig. S18: Optimized geometries of ***EEE*-T1**, ***EEZ*-T1**, ***EZZ*-T1** and ***ZZZ*-T1**and their relative energies (kcal/mol) at B3LYP/6-311G(d,p) level of theory.

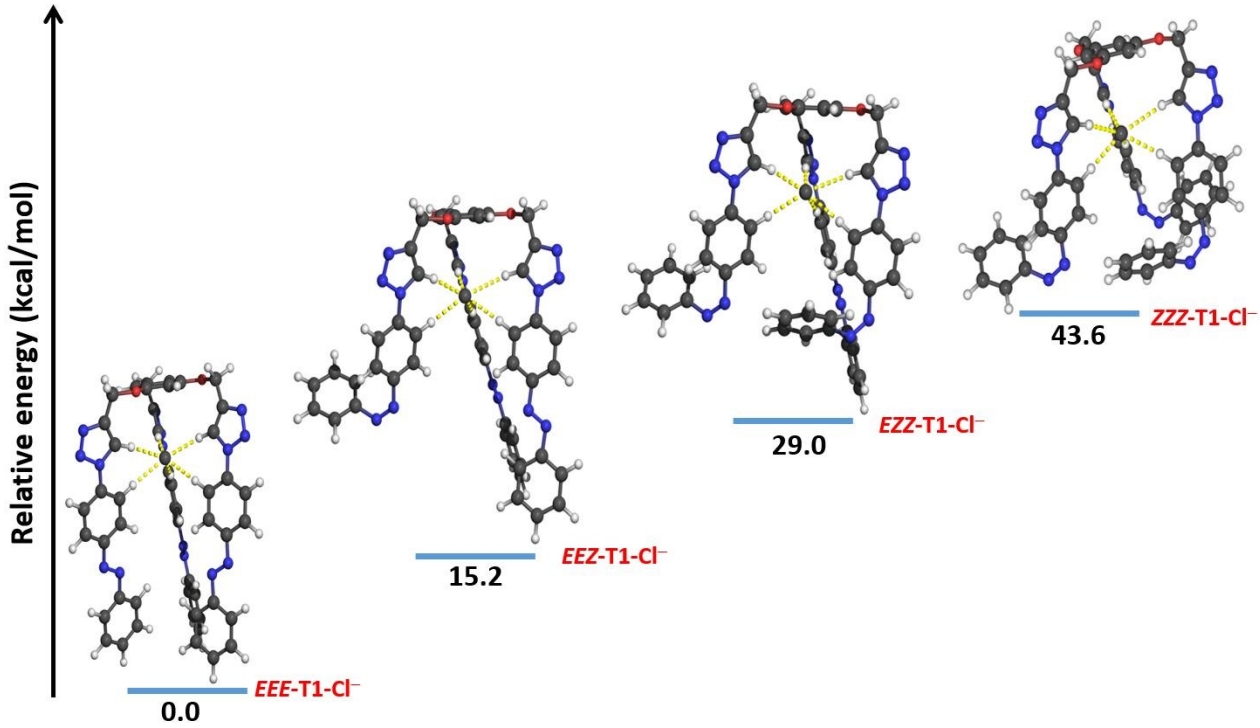


Fig. S19: Optimized geometries of complexes ***EEE*-T1-Cl$^-$**, ***EEZ*-T1-Cl$^-$**, ***EZZ*-T1-Cl$^-$** and ***ZZZ*-T1-Cl$^-$** and their relative energies (kcal/mol) at B3LYP/6-311G(d,p) level of theory.

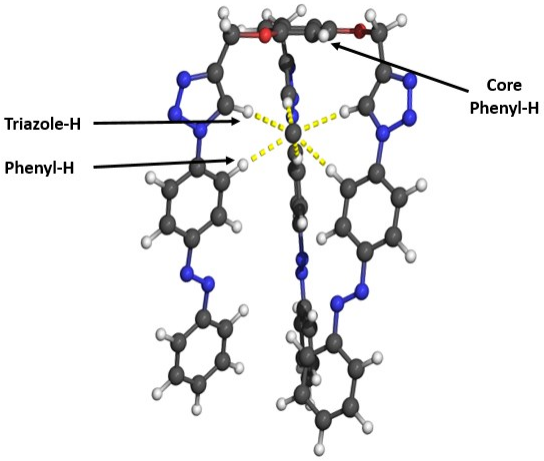
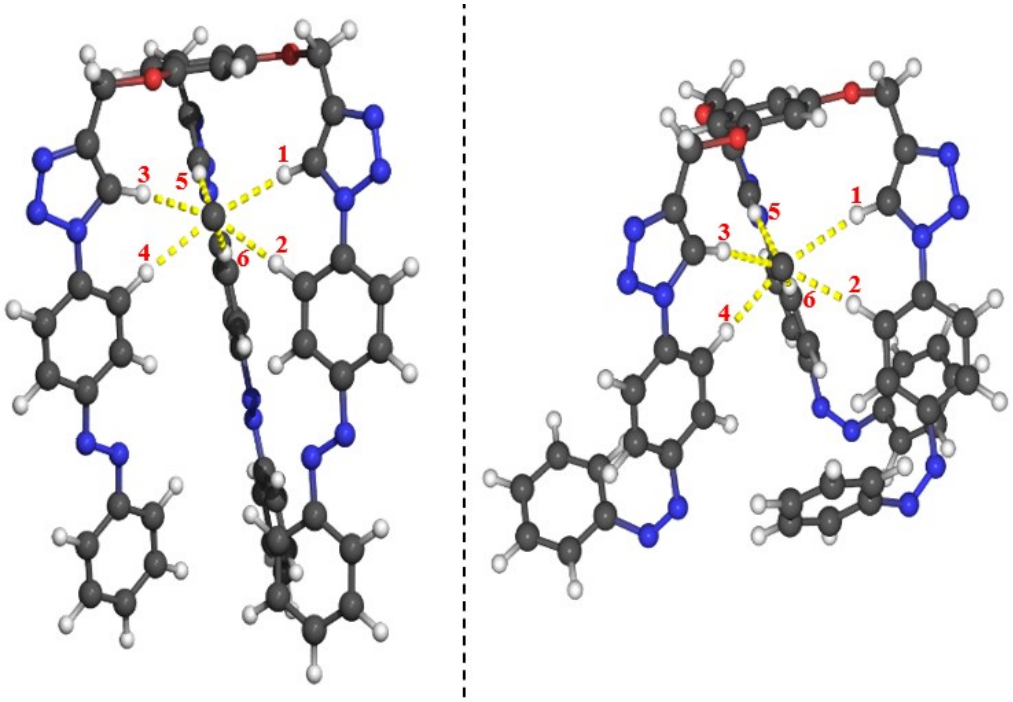


Table S5: Computed Mulliken charges forthe selected hydrogen's in ***EEE*-T1**, ***EEZ*-T1**, ***EZZ*-T1** and ***ZZZ*-T1** and their complexes with Cl^-using B3LYP/6-311G(d,p)) calculations

S.No	Species	Mulliken Charges (atomic units)			
		Triazole-H	Phenyl-H	Core Phenyl-H	Cl^-ion
1	***EEE*-T1**	0.134, 0.132, 0.132	0.118, 0.118, 0.118	0.125, 0.125, 0.128	–
2	***EEE*-T1**–Cl^-	0.218, 0.212, 0.211	0.198, 0.191, 0.200	0.101, 0.100, 0.104	–0.886
3	***EEZ*-T1**	0.138, 0.134, 0.132	0.125, 0.120, 0.118	0.126, 0.121, 0.123	
4	***EEZ*-T1**–Cl^-	0.220, 0.215, 0.210	0.202, 0.199, 0.192	0.105, 0.104, 0.100	–0.890
5	***EZZ*-T1**	0.133, 0.131, 0.130	0.115, 0.115, 0.114	0.126, 0.124, 0.123	–
6	***EZZ*-T1**–Cl^-	0.223, 0.213, 0.207	0.203, 0.189, 0.197	0.105, 0.103, 0.098	–0.890
7	***ZZZ*-T1**	0.133, 0.131, 0.129	0.116, 0.116, 0.112	0.130, 0.124, 0.117	–
8	***ZZZ*-T1**–Cl^-	0.216, 0.211, 0.211	0.199, 0.199, 0.196	0.105, 0.103, 0.105	–0.892



***EEE*-Cl⁻** ***ZZZ*-Cl⁻**

Table S6: The second order perturbation orbital interaction energies (in kcal/mol) from the natural bond orbital (NBO) analysis in *EEE-Cl⁻* and *ZZZ-Cl⁻* isomers at M06-2X/6-311G(d,p) level of theory.

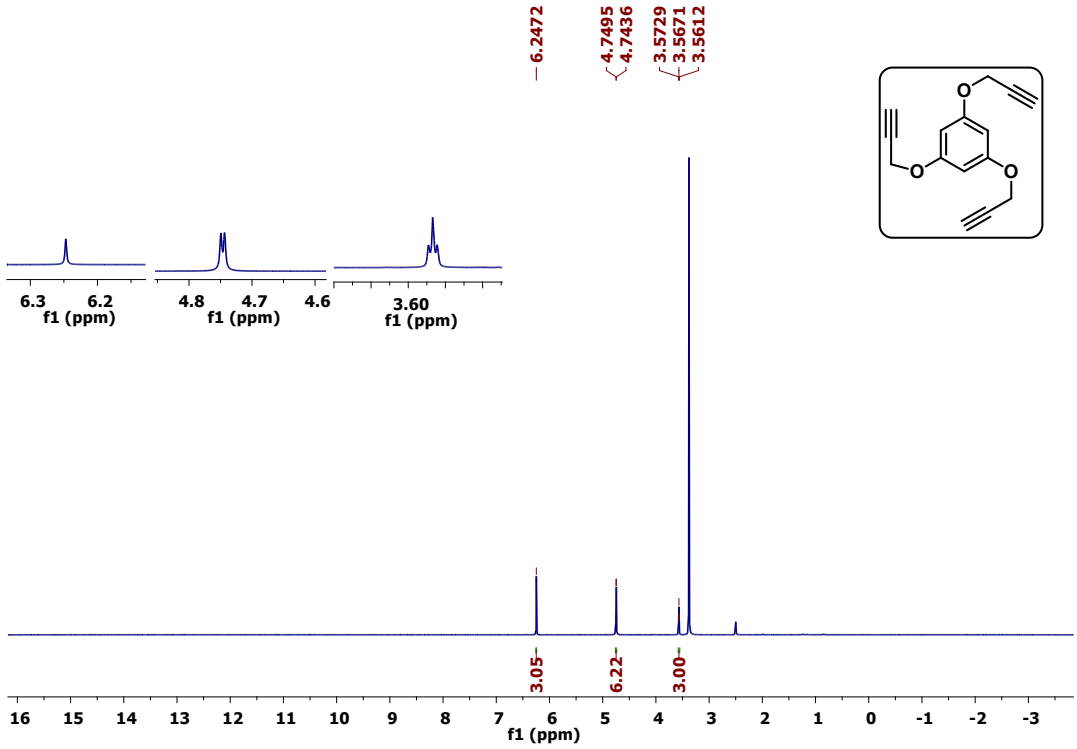
Species	Donor	Acceptor	E (kcal/mol)	Species	Donor	Acceptor	E (kcal/mol)
EEE-Cl⁻	n_{Cl-}	$\sigma^*_{(1H-C)}$	10.2	ZZZ-Cl⁻	n_{Cl-}	$\sigma^*_{(1H-C)}$	6.9
	n_{Cl-}	$\sigma^*_{(2H-C)}$	6.1		n_{Cl-}	$\sigma^*_{(2H-C)}$	3.0
	n_{Cl-}	$\sigma^*_{(3H-C)}$	8.5		n_{Cl-}	$\sigma^*_{(3H-C)}$	7.5
	n_{Cl-}	$\sigma^*_{(4H-C)}$	6.0		n_{Cl-}	$\sigma^*_{(4H-C)}$	5.3
	n_{Cl-}	$\sigma^*_{(5H-C)}$	9.6		n_{Cl-}	$\sigma^*_{(5H-C)}$	7.6
	n_{Cl-}	$\sigma^*_{(6H-C)}$	4.3		n_{Cl-}	$\sigma^*_{(6H-C)}$	5.4

Table S7: Computational data of ***EEE*-T1**, ***EEZ*-T1**, ***EZZ*-T1** and ***ZZZ*-T1** and their complexes with F^-, Cl^- and Br^- at B3LYP/6-311G(d,p) level of theory.

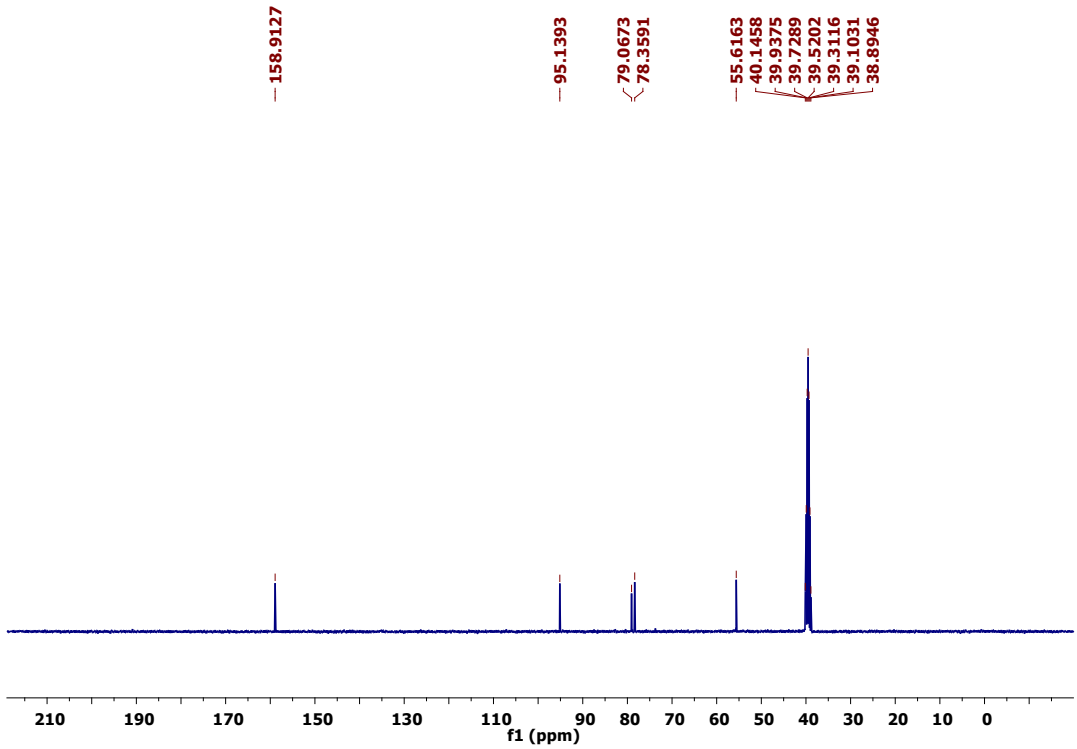
Species	Electronic energy[a] (Hartrees)	Enthalpy[a] (H) (Hartrees)	Free Energy[a] (G) (Hartrees)	Lowest frequency (cm^{-1})	Point Group	Electronic State
F^-	–99.821335	–99.818975	–99.835494	–	O_h	$^1A_{1g}$
Cl^-	–460.300710	–460.298350	–460.315733	–	O_h	$^1A_{1g}$
Br^-	–2574.227931	–2574.225571	–2574.244107	–	O_h	$^1A_{1g}$
***EEE*-T1**	–3013.492590	–3013.435604	–3013.594565	8.62	C_1	^1A
***EEE*-T1**–F^-	–3113.486348	–3113.428122	–3113.587910	6.62	C_1	^1A
***EEE*-T1**–Cl^-	–3473.861092	–3473.801929	–3473.967424	6.49	C_1	^1A
***EEE*-T1**–Br^-	–5587.784522	–5587.724983	–5587.894295	4.25	C_1	^1A
***EEZ*-T1**	–3013.465959	–3013.408833	–3013.568932	7.00	C_1	^1A
***EEZ* -T1**–F^-	–3113.461586	–3113.403272	–3113.565880	4.12	C_1	^1A
***EEZ*-T1** –Cl^-	–3473.836860	–3473.777500	–3473.946244	3.93	C_1	^1A
***EEZ* -T1**–Br^-	–5587.761516	–5587.702021	–5587.869551	5.99	C_1	^1A
***EZZ*-T1**	–3013.442671	–3013.385546	–3013.545260	9.78	C_1	^1A
***EZZ*-T1**–F^-	–3113.438347	–3113.380249	–3113.539498	7.87	C_1	^1A
***EZZ*-T1**–Cl^-	–3473.814870	–3473.755783	–3473.920498	4.73	C_1	^1A
***EZZ*-T1**–Br^-	–5587.738029	–5587.678643	–5587.845534	4.18	C_1	^1A
***ZZZ*-T1**	–3013.419830	–3013.362736	–3013.523673	3.72	C_1	^1A
***ZZZ*-T1**–F^-	–3113.412835	–3113.354737	–3113.514218	6.46	C_1	^1A
***ZZZ*-T1**–Cl^-	–3473.791569	–3473.732599	–3473.895694	7.99	C_1	^1A
***ZZZ*-T1**–Br^-	–5587.715366	–5587.656076	–5587.821382	7.59	C_1	^1A

[a]Zero-point corrected electronic energies (E), enthalpies and free energies (G) of ***EEE*-T1**, ***EEZ*-T1**, ***EZZ*-T1** and ***ZZZ*-T1** and their complexes with F^-, Cl^- and Br^- (in Hartrees) at B3LYP/6-311G(d,p) level of theory.

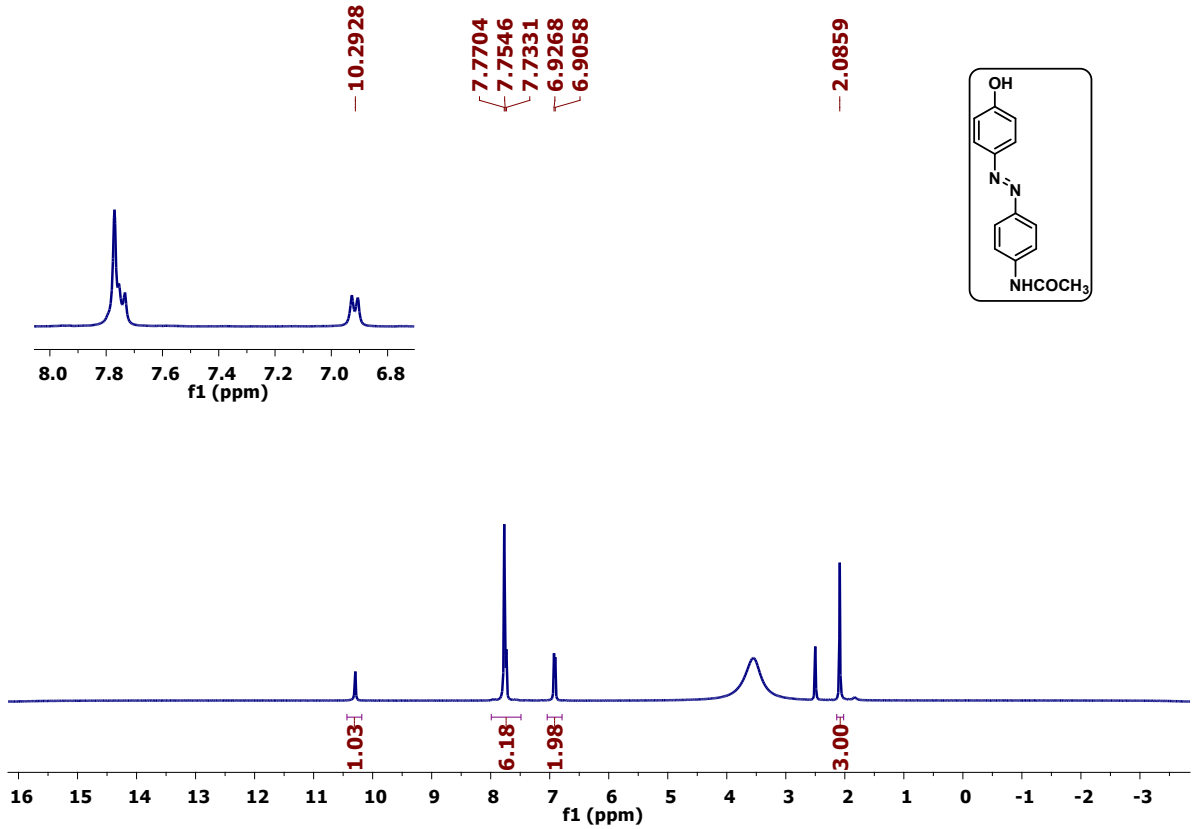
S12. Spectral characterization data (^{1}H- and ^{13}C-NMR data)



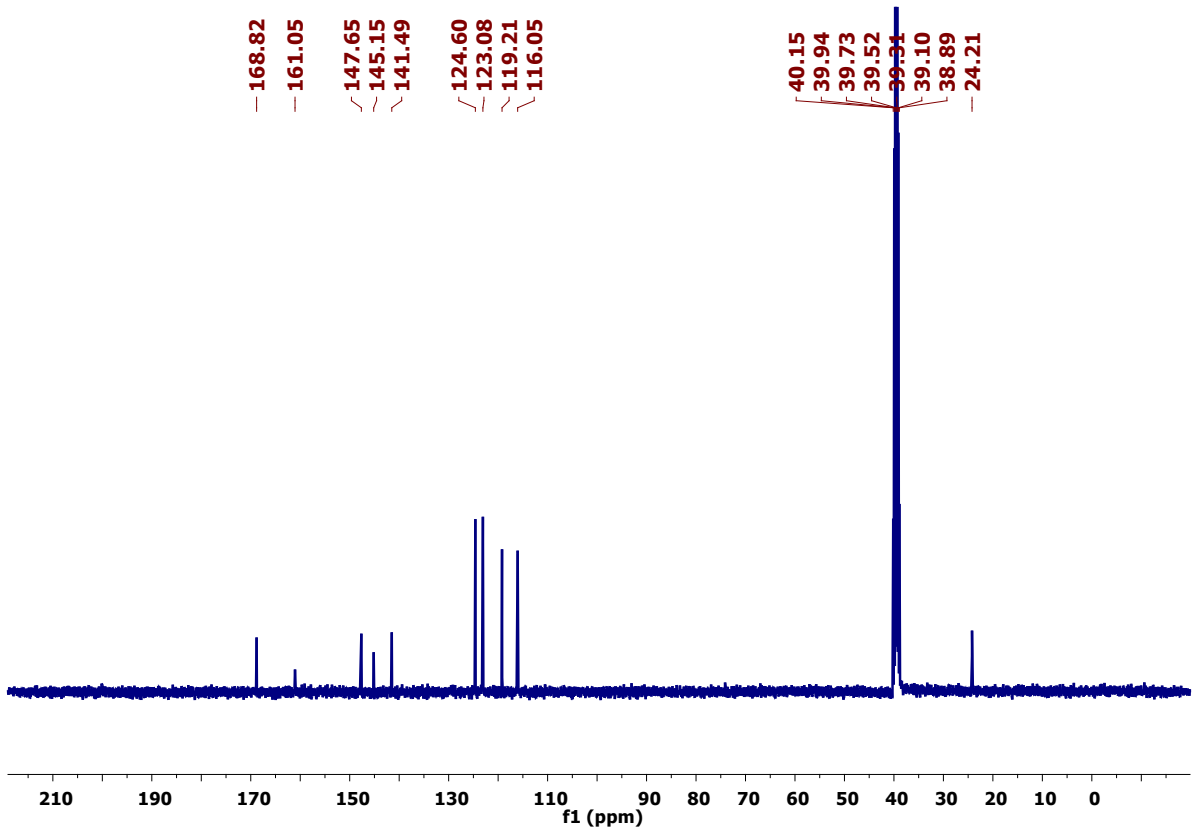
^{1}H NMR spectrum of 1,3,5-*tris*(prop-2-yn-1-yloxy)benzene (**C1**) in DMSO-d_6



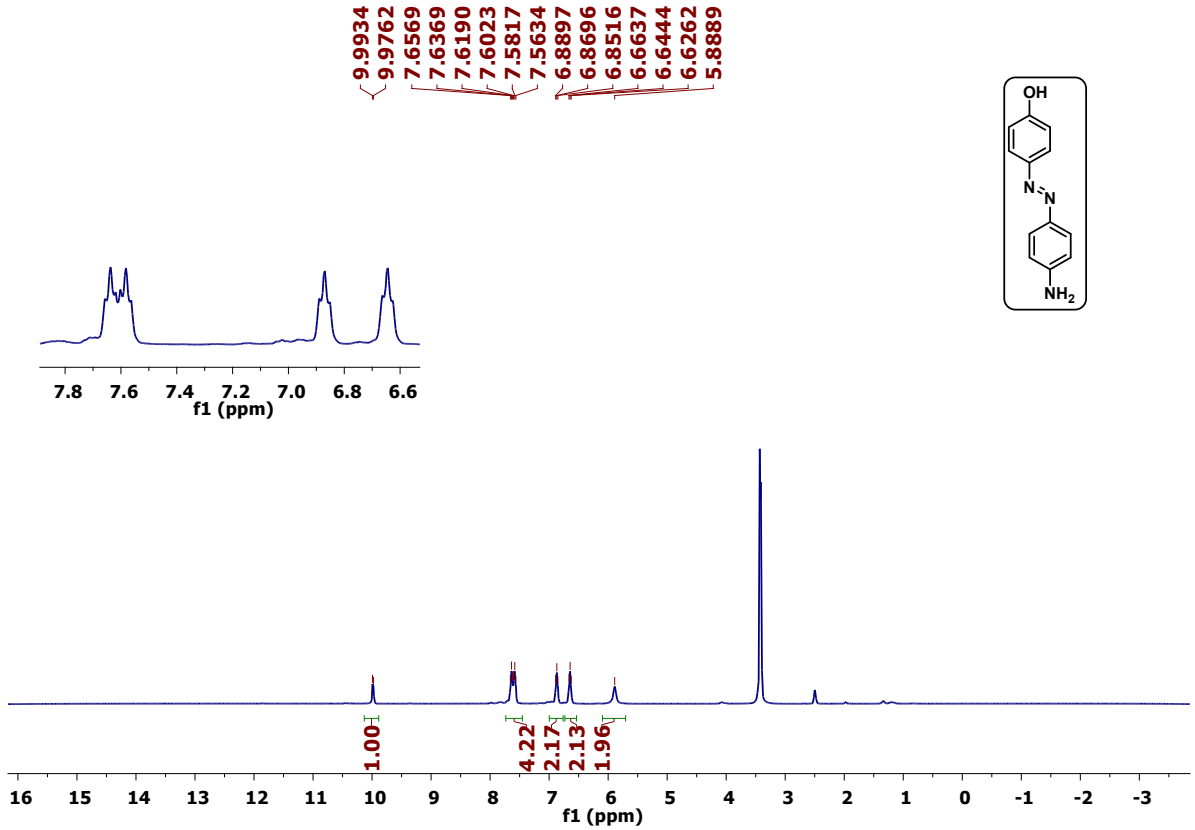
^{13}C NMR spectrum of 1,3,5-*tris*(prop-2-yn-1-yloxy)benzene (**C1**) in DMSO-d_6



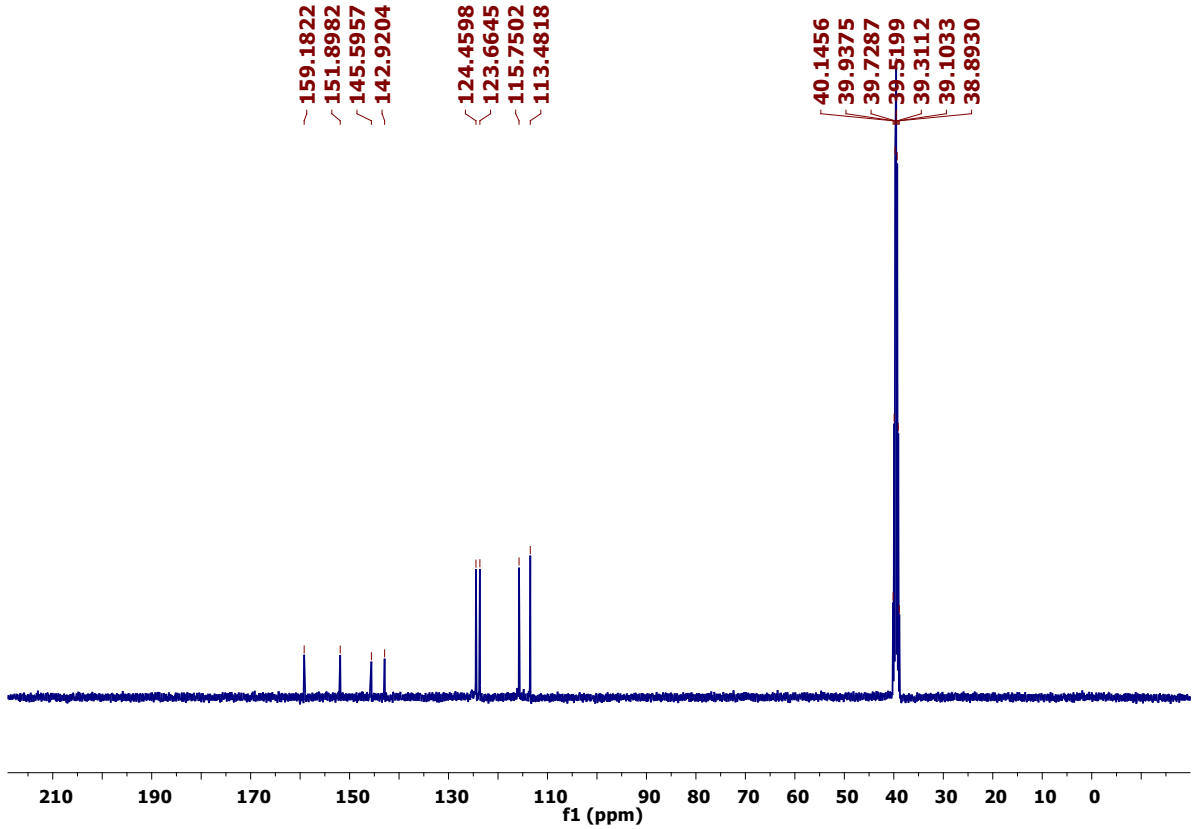
^{1}H NMR spectrum of *(E)*-N-(4-((4-hydroxyphenyl)diazenyl)phenyl)acetamide(**3**) in DMSO-d_6



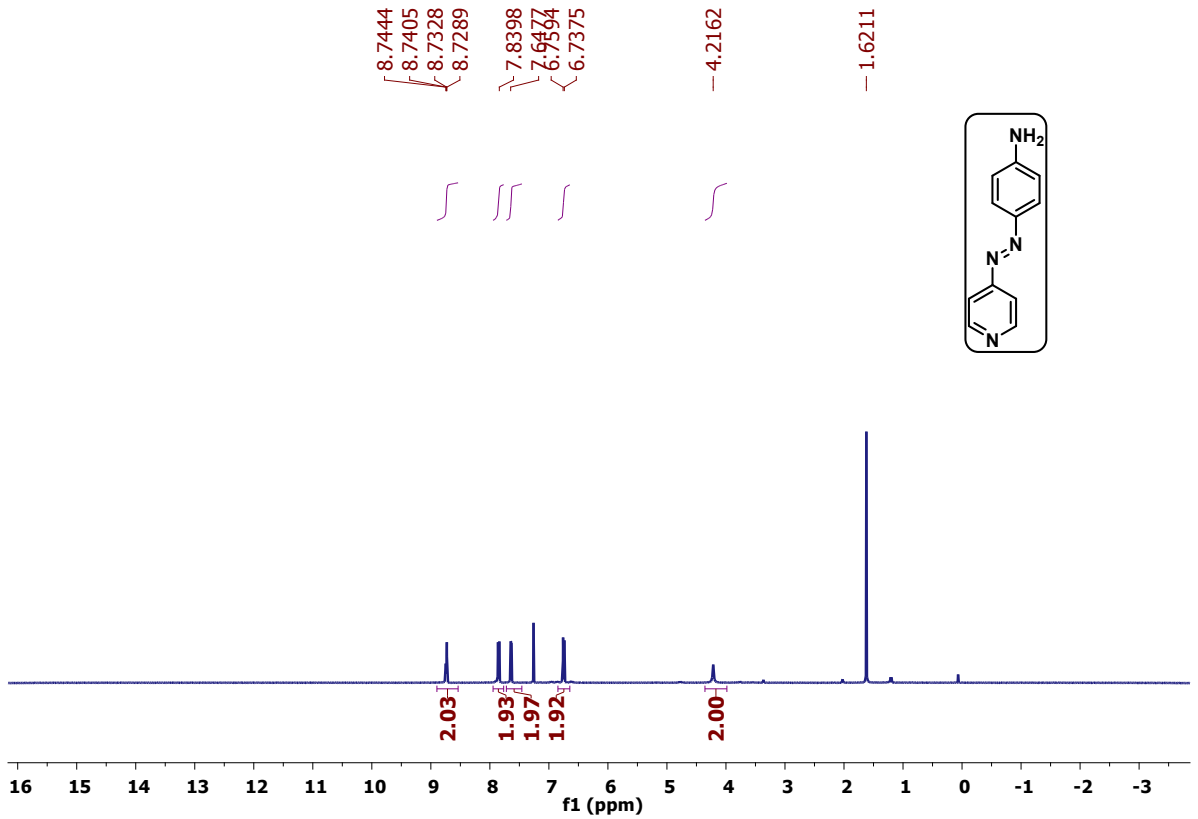
^{13}C NMR spectrum of *(E)*-N-(4-((4-hydroxyphenyl)diazenyl)phenyl)acetamide(**3**) in DMSO-d_6



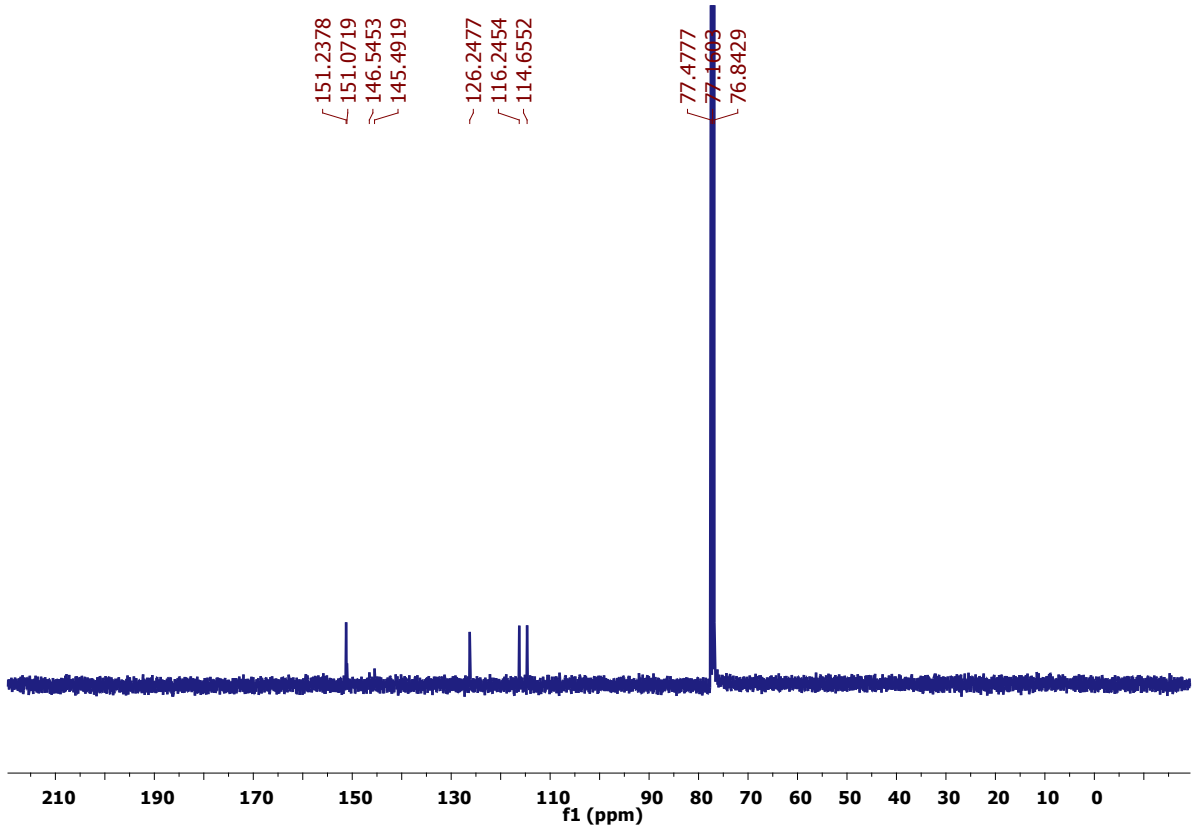
^{1}H NMR spectrum of (*E*)-4-((4-aminophenyl)diazenyl)phenol(**Am2**)in DMSO-d_6



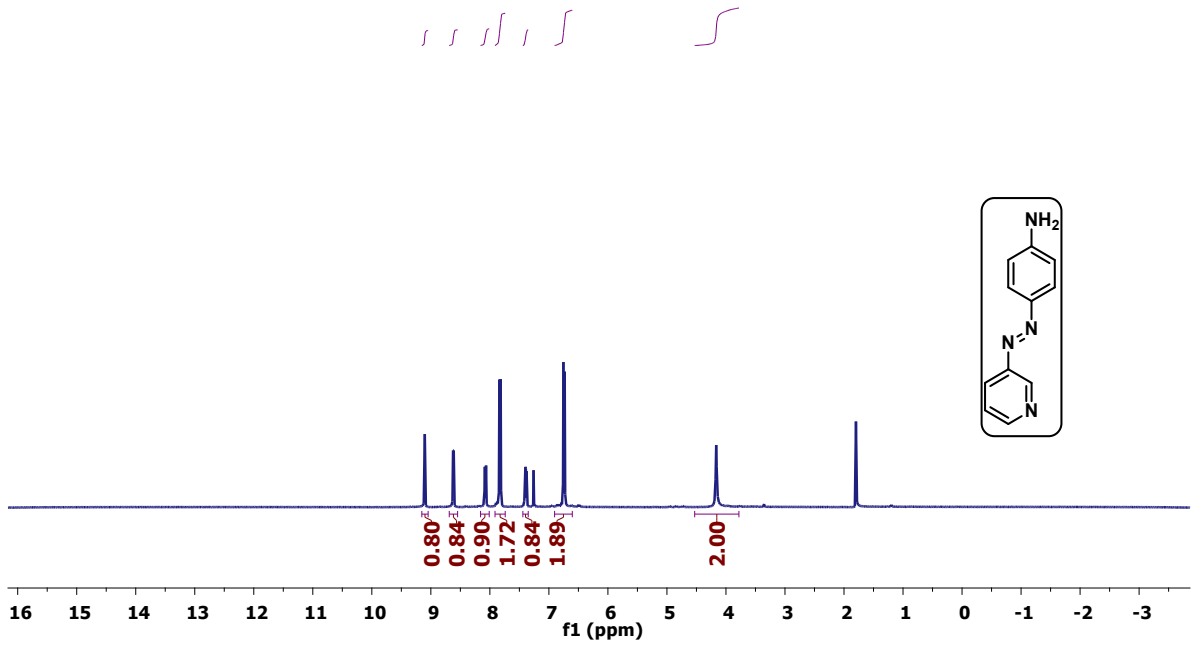
^{13}C NMR spectrum of (*E*)-4-((4-aminophenyl)diazenyl)phenol(**Am2**)in DMSO-d_6



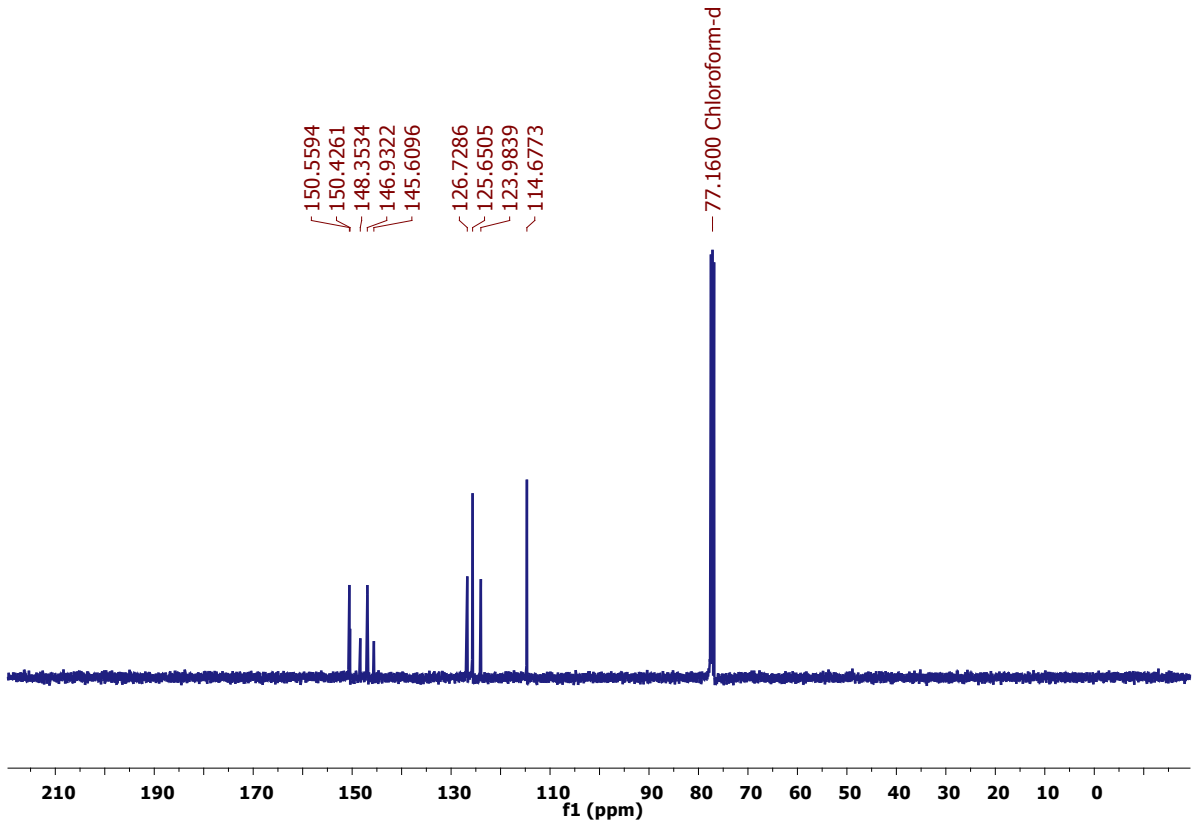
^{1}H NMR spectrum of (*E*)-4-(pyridin-4-yldiazenyl)aniline(**Am3**)in $CDCl_3$



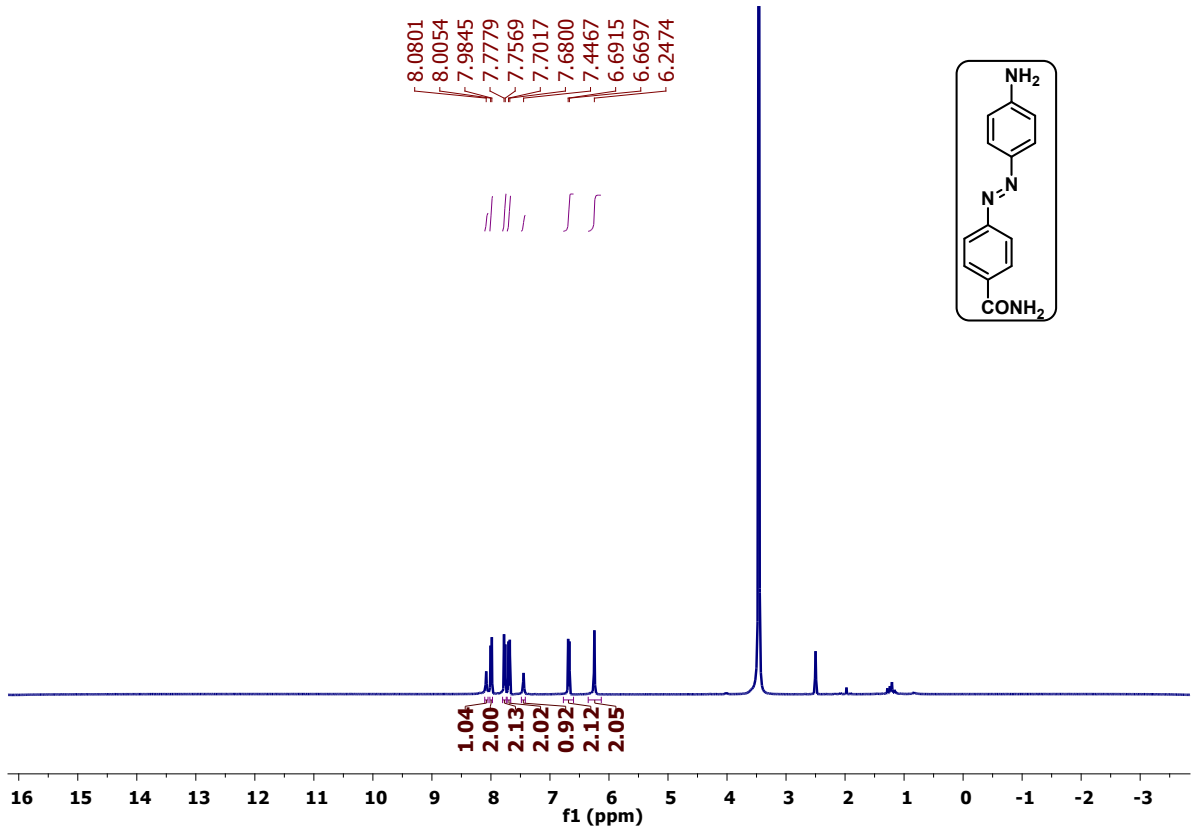
^{13}C NMR spectrum of (*E*)-4-(pyridin-4-yldiazenyl)aniline(**Am3**)in $CDCl_3$



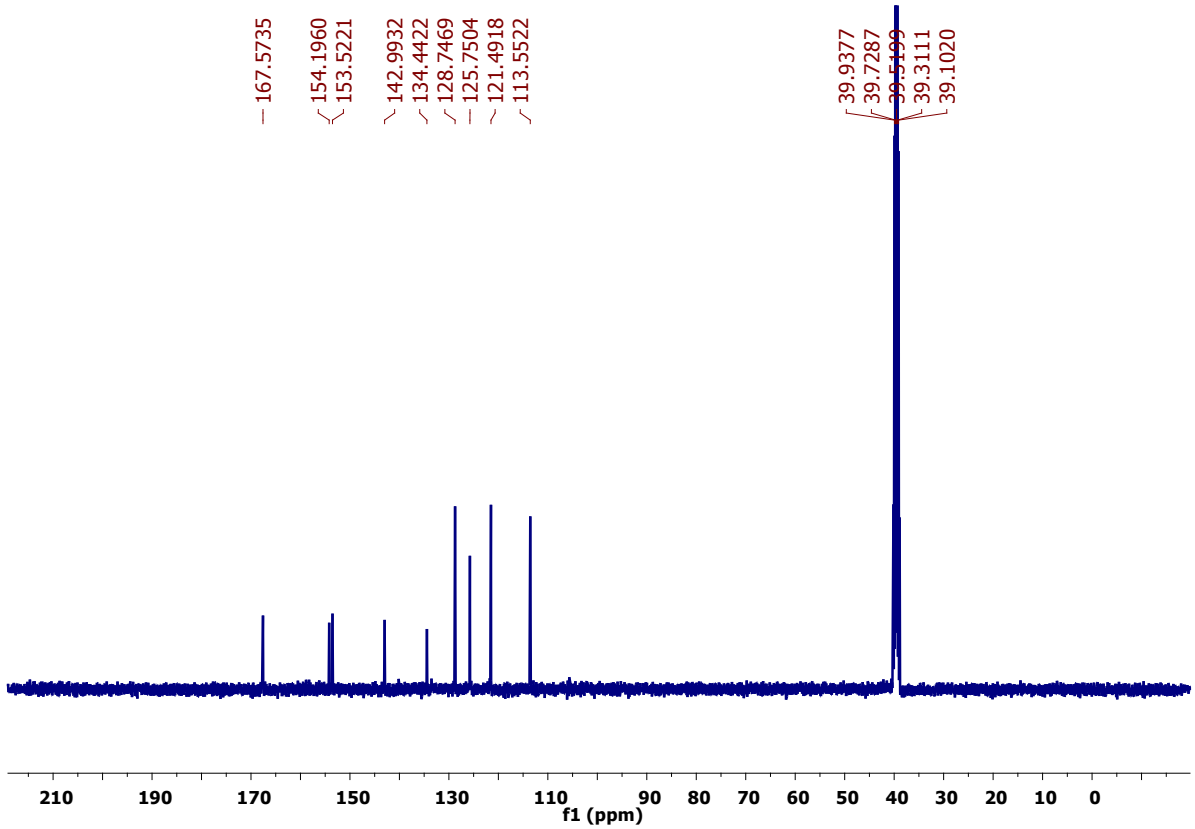
^{1}H NMR spectrum of (*E*)-4-(pyridin-3-yldiazenyl)aniline(**Am4**)in $CDCl_3$



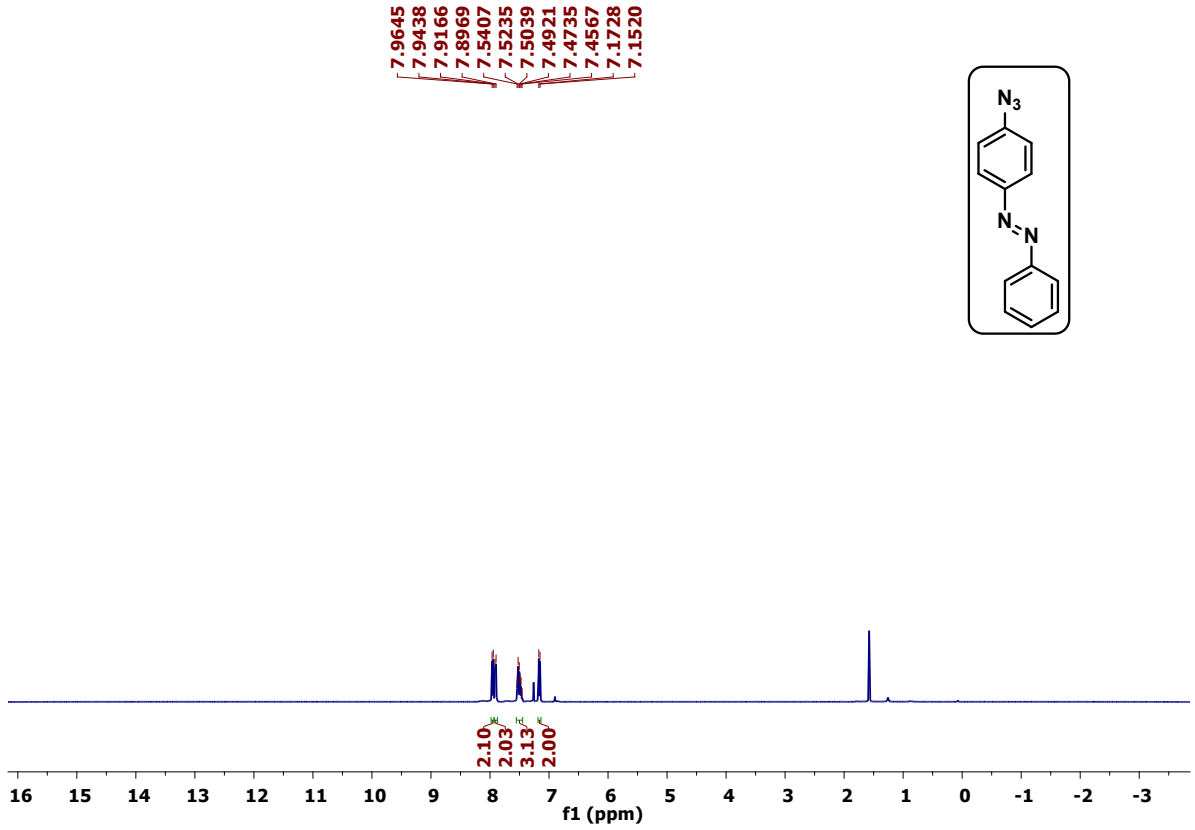
^{13}C NMR spectrum of (*E*)-4-(pyridin-3-yldiazenyl)aniline(**Am4**)in $CDCl_3$



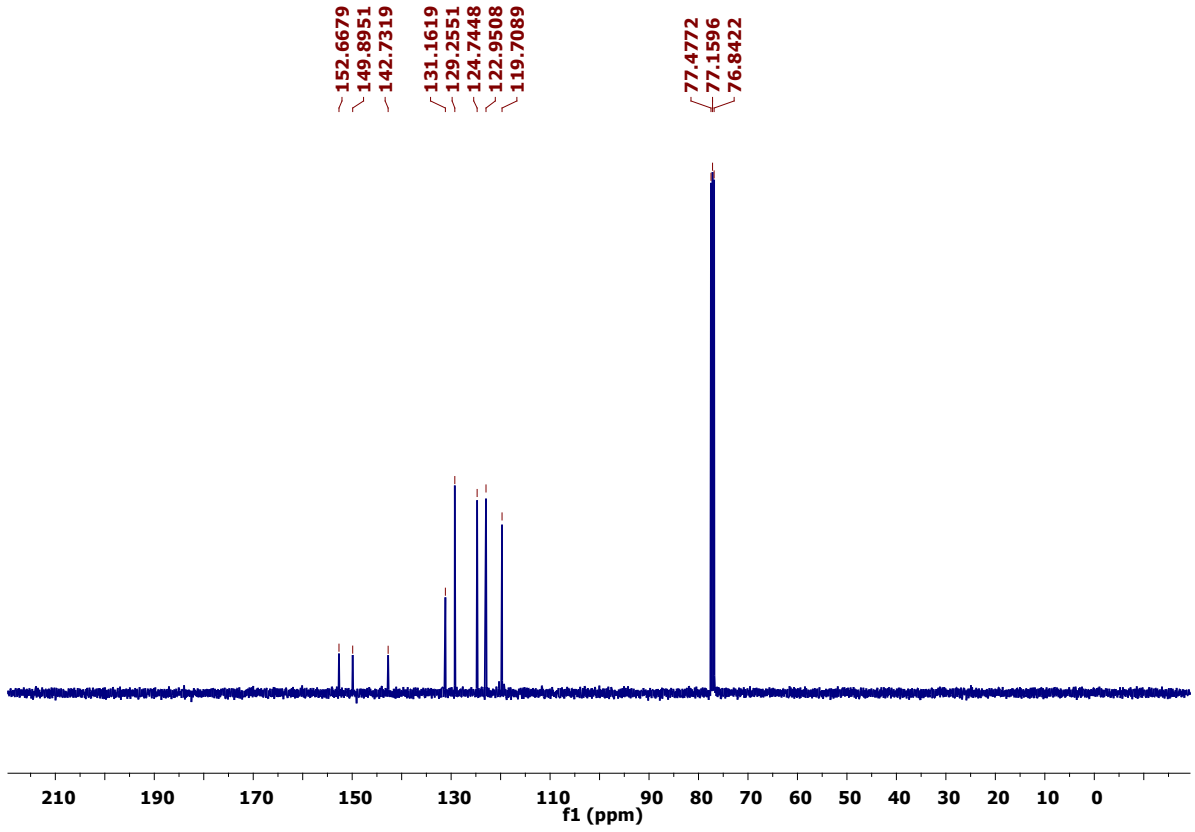
^{1}H NMR spectrum of (*E*)-4-((4-aminophenyl)diazenyl)benzamide (**Am5**) in DMSO-d_6



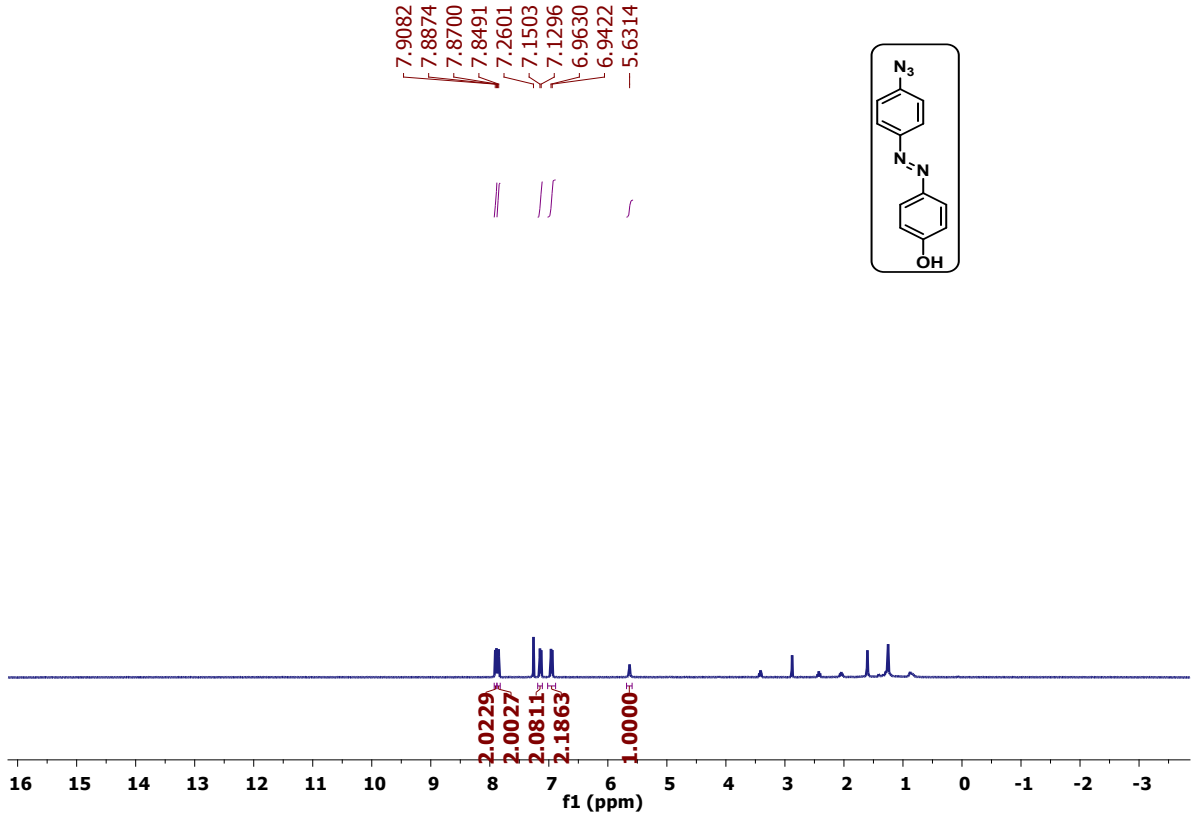
^{13}C NMR spectrum of (*E*)-4-((4-aminophenyl)diazenyl)benzamide (**Am5**) in DMSO-d_6



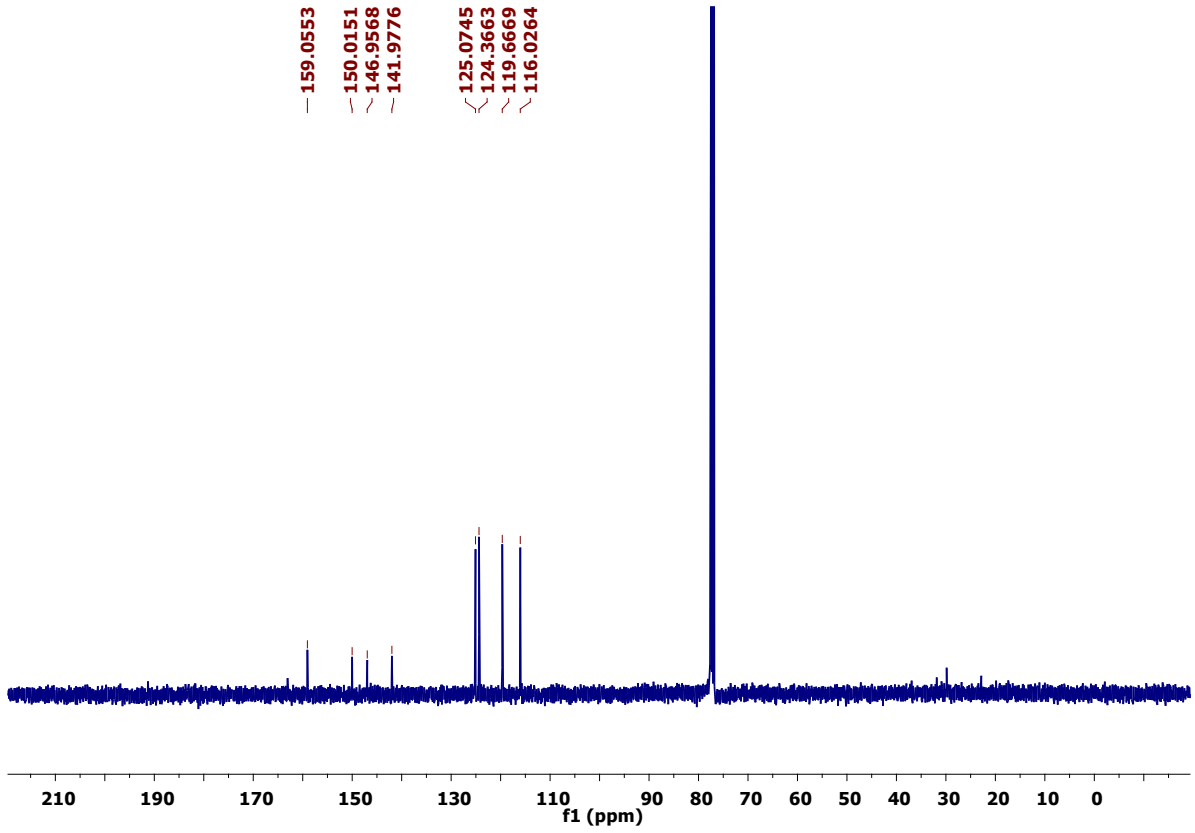
^{1}H NMR spectrum of (*E*)-1-(4-azidophenyl)-2-phenyldiazene (**Az1**)in $CDCl_3$



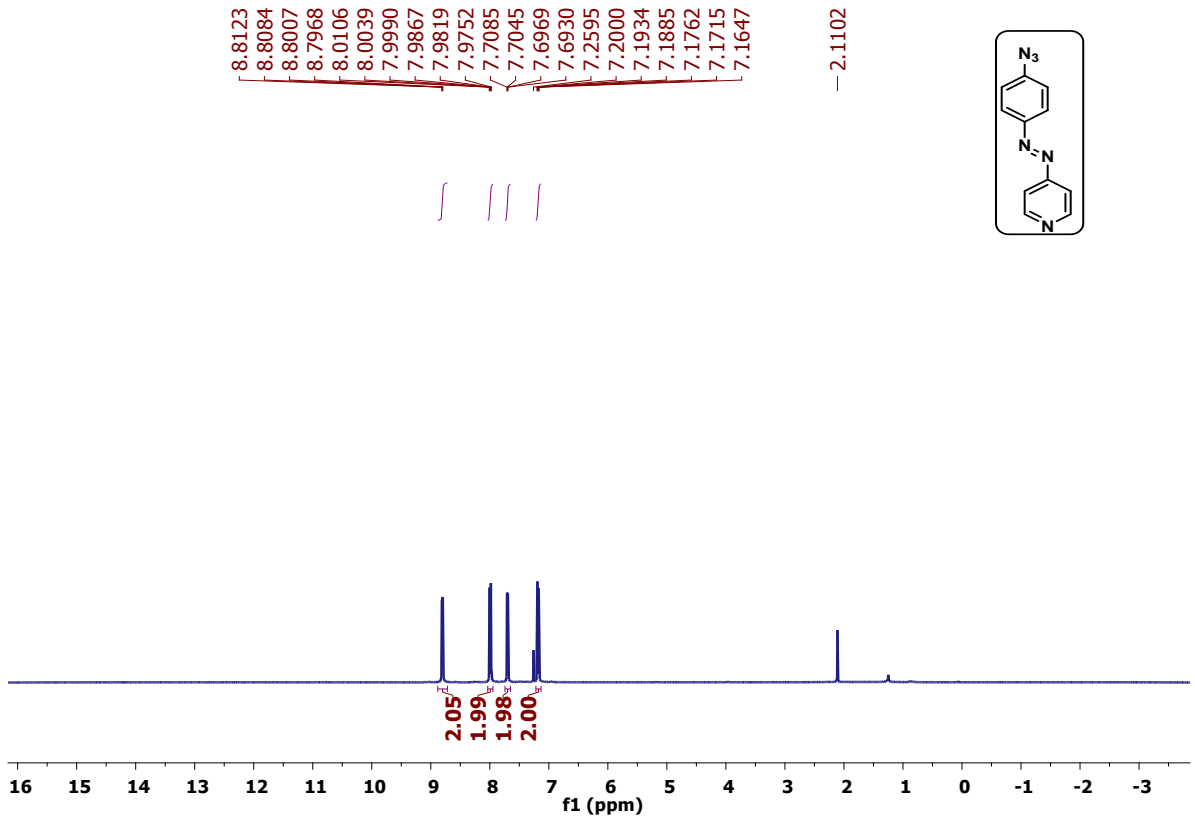
^{13}C NMR spectrum of (*E*)-1-(4-azidophenyl)-2-phenyldiazene (**Az1**)in $CDCl_3$



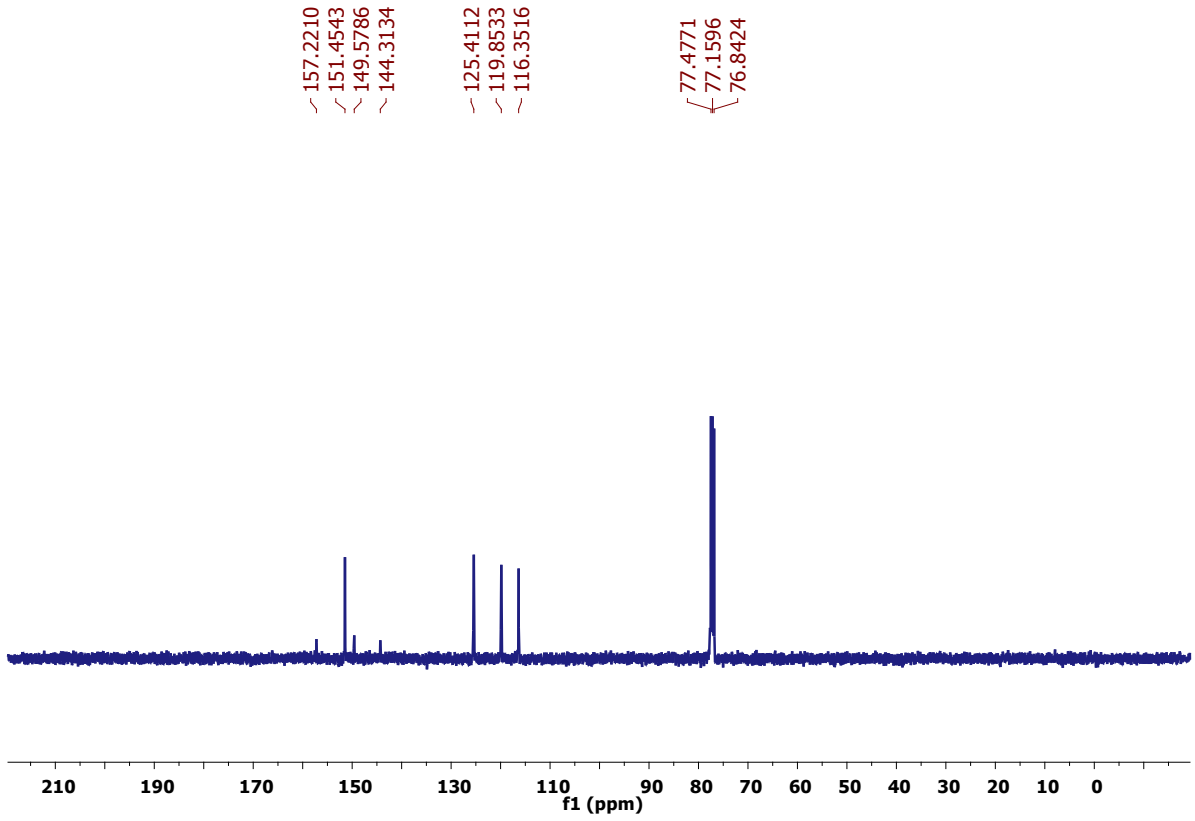
^{1}H NMR spectrum of (*E*)-4-((4-azidophenyl)diazenyl)phenol (**Az2**)in $CDCl_3$



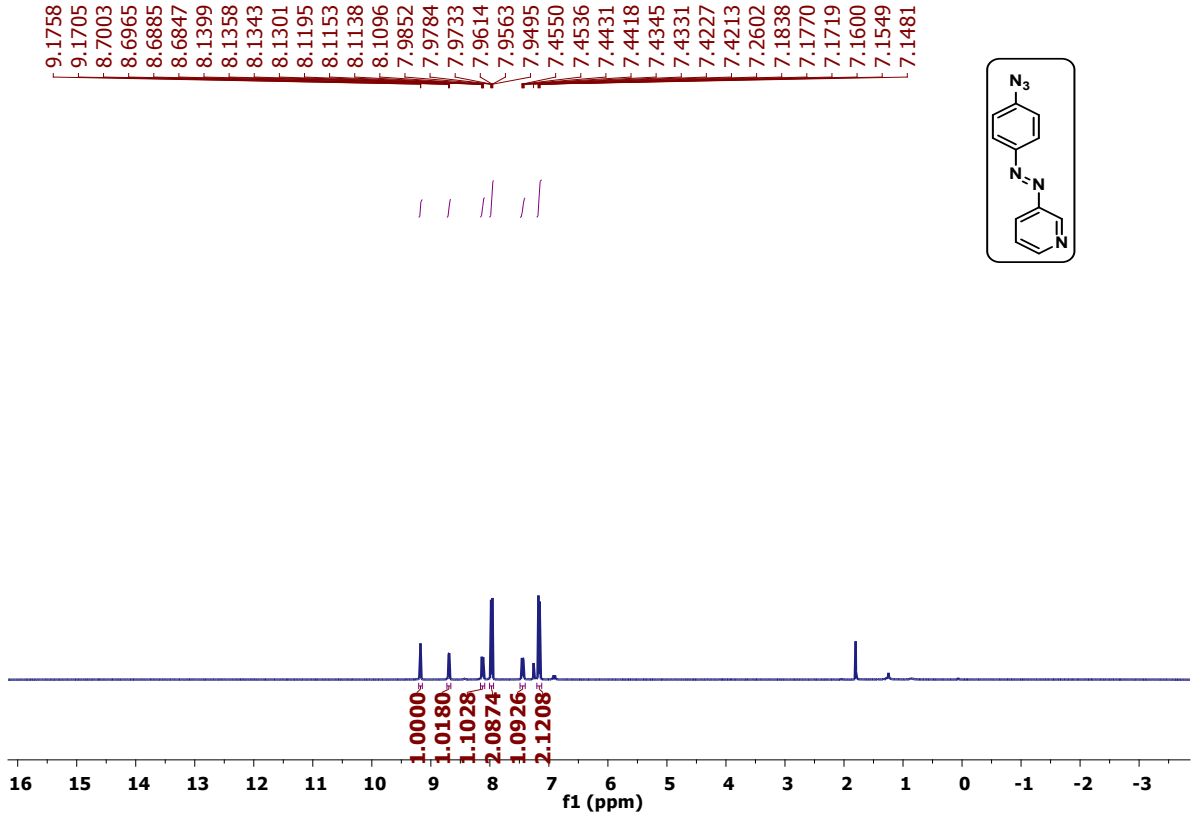
^{13}C NMR spectrum of (*E*)-4-((4-azidophenyl)diazenyl)phenol (**Az2**)in $CDCl_3$



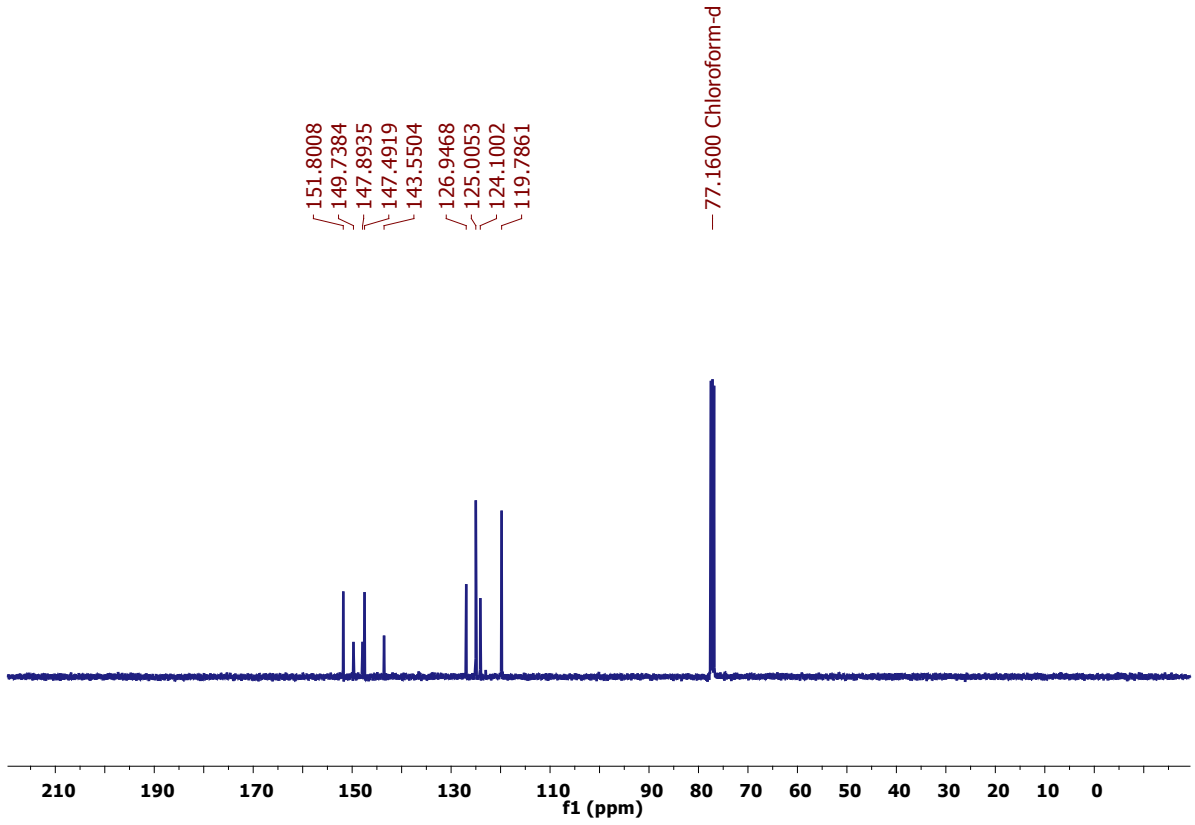
^{1}H NMR spectrum of (*E*)-4-((4-azidophenyl)diazenyl)pyridine (**Az3**)in $CDCl_3$



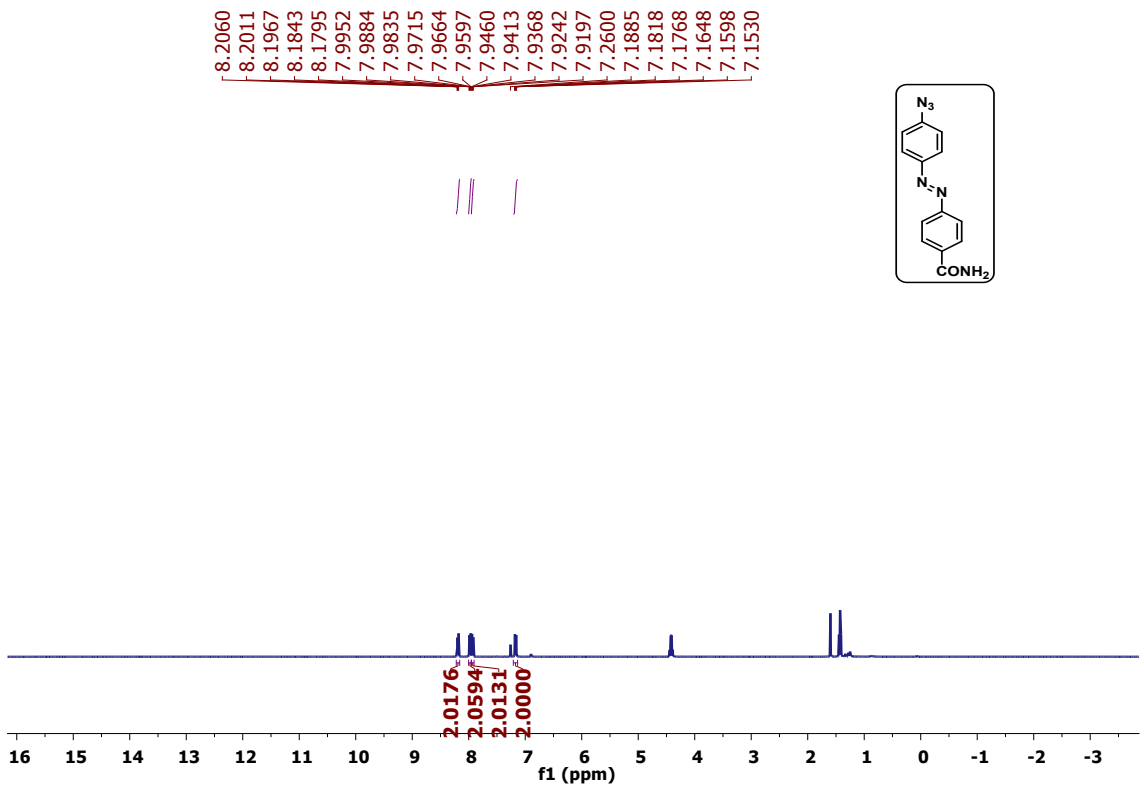
^{13}C NMR spectrum of (*E*)-4-((4-azidophenyl)diazenyl)pyridine (**Az3**)in $CDCl_3$



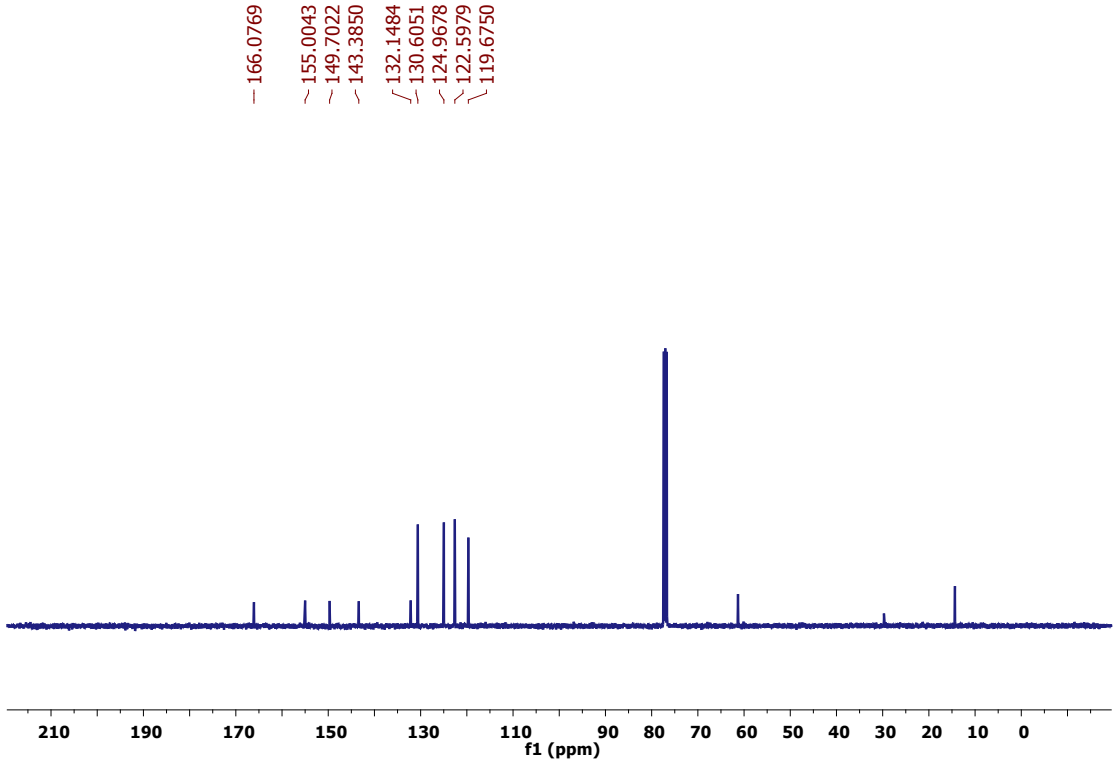
^{1}H NMR spectrum of (*E*)-3-((4-azidophenyl)diazenyl)pyridine (**Az4**)in $CDCl_3$



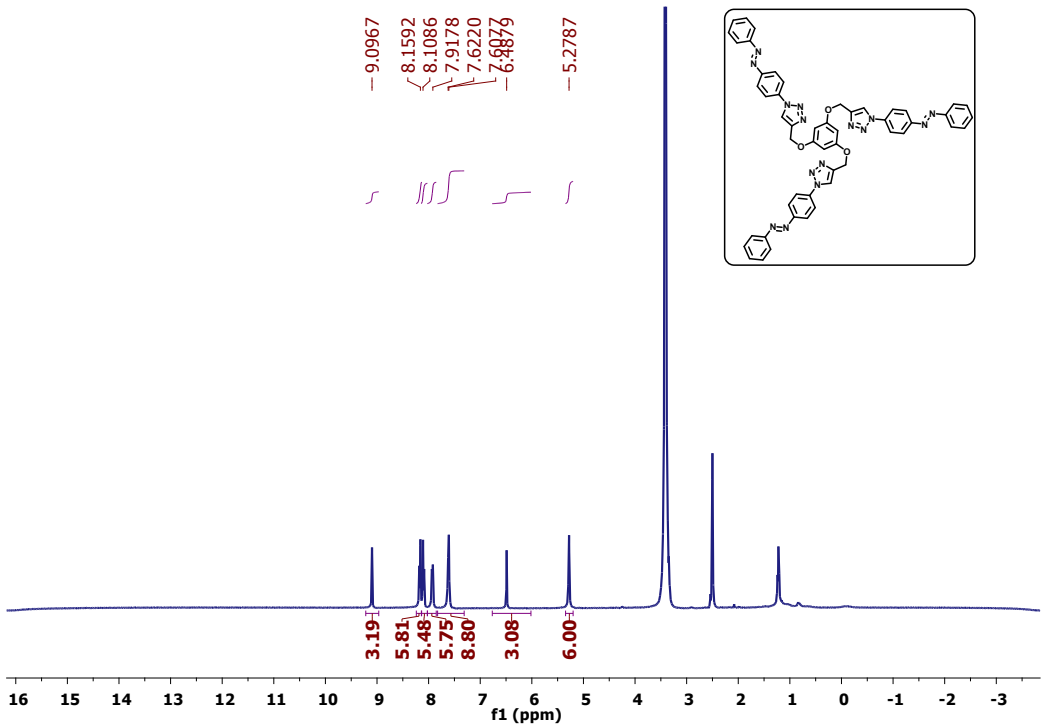
^{13}C NMR spectrum of (*E*)-3-((4-azidophenyl)diazenyl)pyridine (**Az4**)in $CDCl_3$



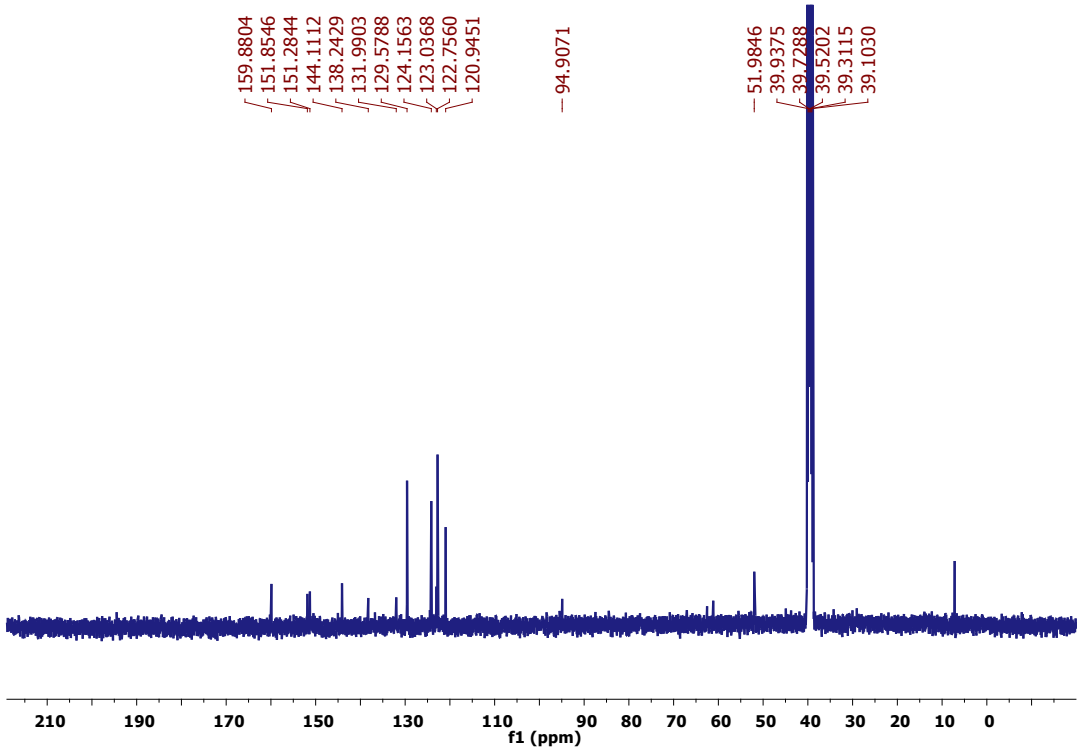
^{1}H NMR spectrum of (*E*)-4-((4-azidophenyl)diazenyl)benzamide(**Az5**)in $CDCl_3$



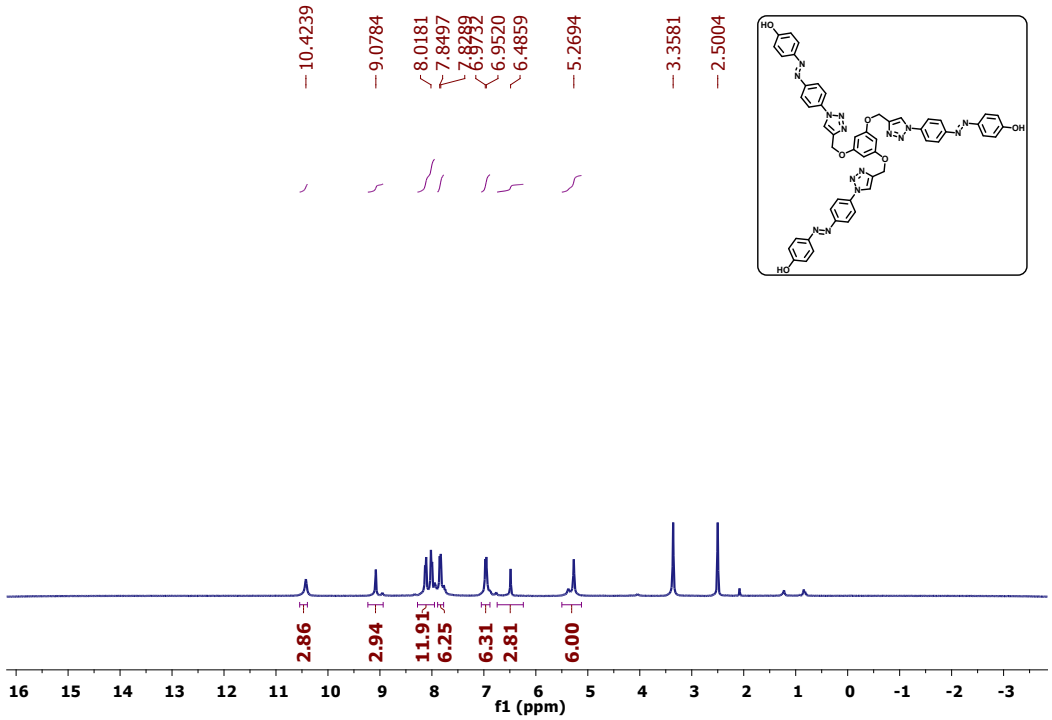
^{13}C NMR spectrum of (*E*)-4-((4-azidophenyl)diazenyl)benzamide(**Az5**)in $CDCl_3$



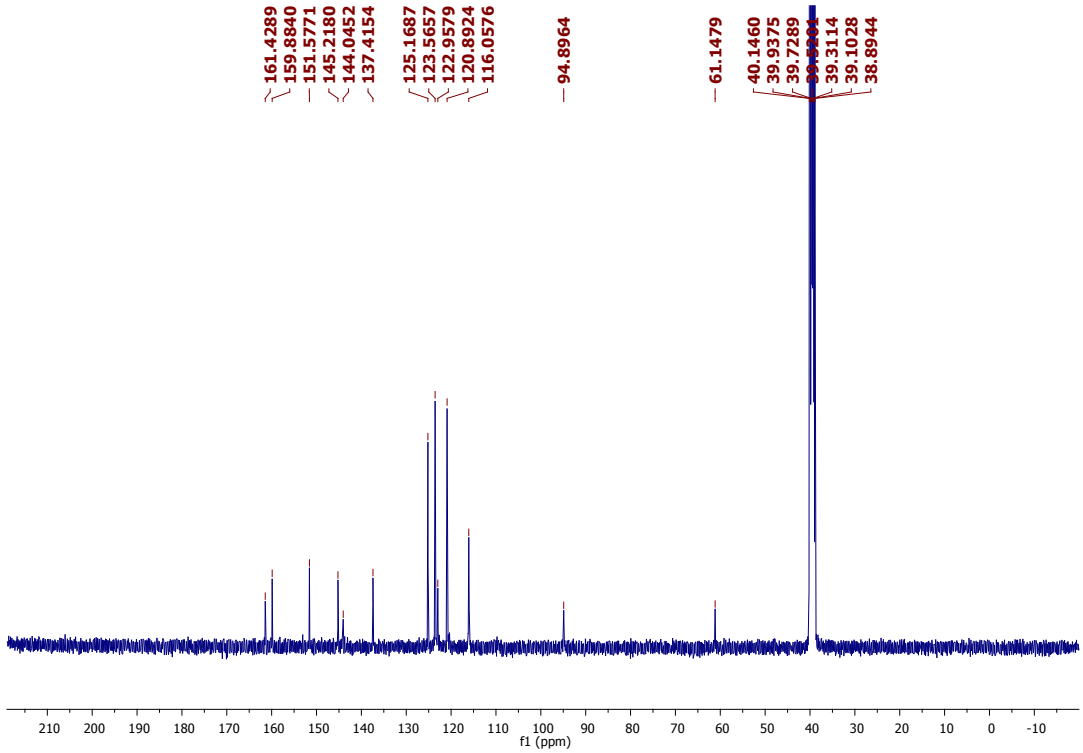
^{1}H NMR spectrum of 4,4'-(((5-((2-(4-((*E*)-phenyldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1-(4-((*E*)-phenyldiazenyl)phenyl)-1*H*-1,2,3-triazole) (**T1**)in DMSO-d_6



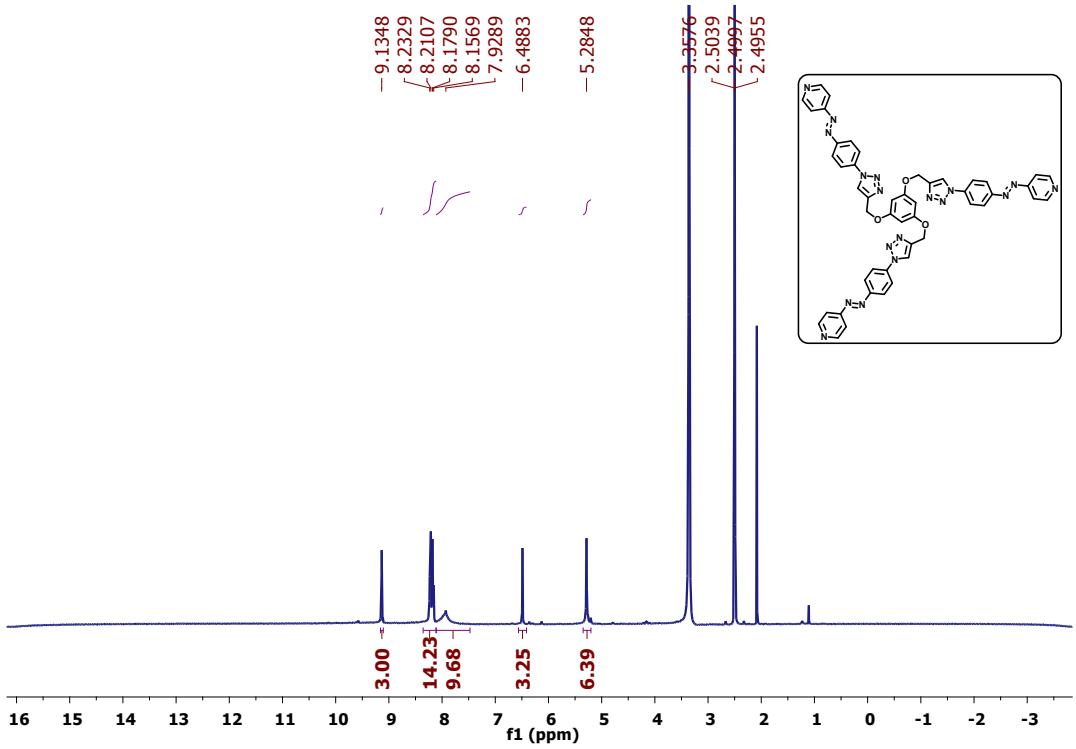
^{13}C NMR spectrum of 4,4'-(((5-((2-(4-((*E*)-phenyldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1-(4-((*E*)-phenyldiazenyl)phenyl)-1*H*-1,2,3-triazole) (**T1**) in DMSO-d_6



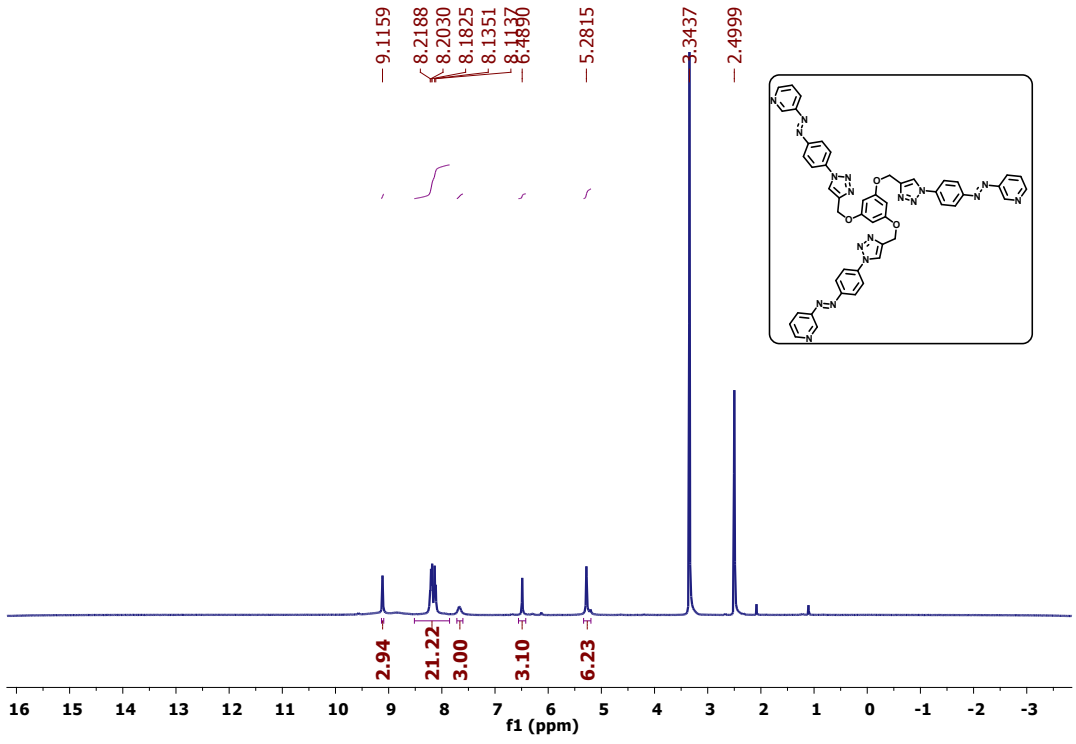
^{1}H NMR spectrum of 4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-(4-hydroxyphenyl)diazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))diphenol (**T2**)in DMSO-d_6



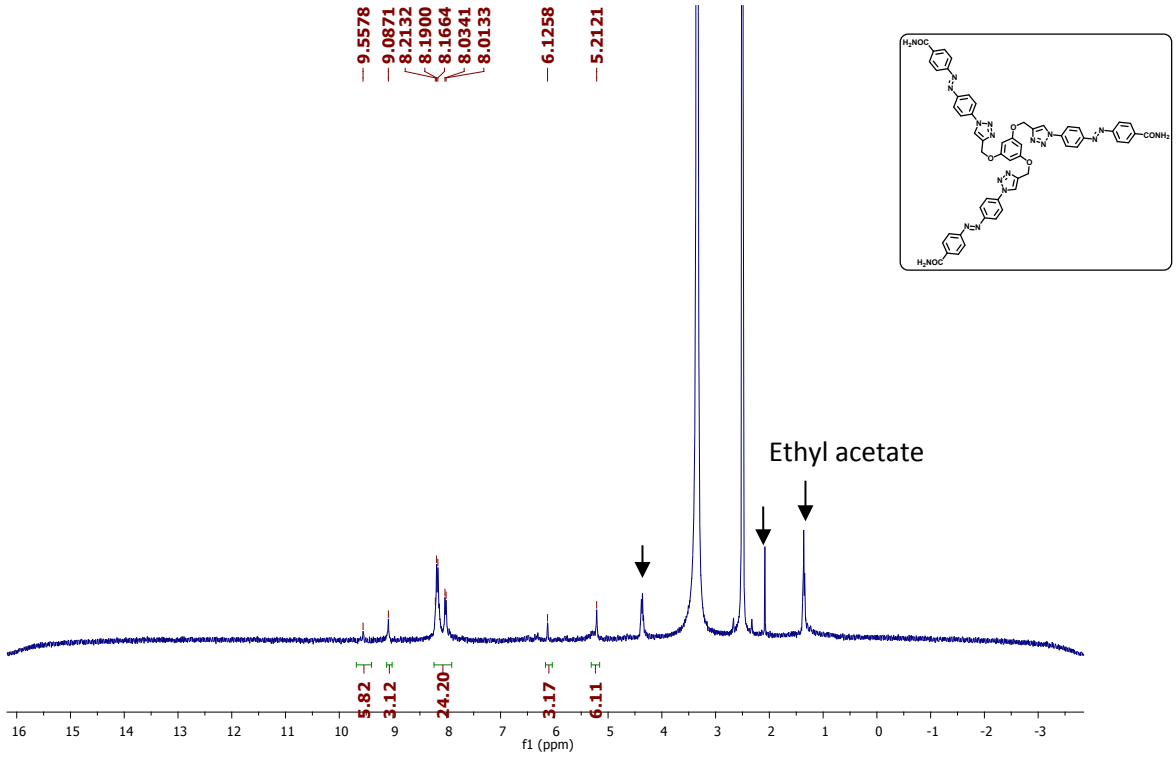
^{13}C NMR spectrum of 4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-(4-hydroxyphenyl)diazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))diphenol (**T2**) in DMSO-d_6



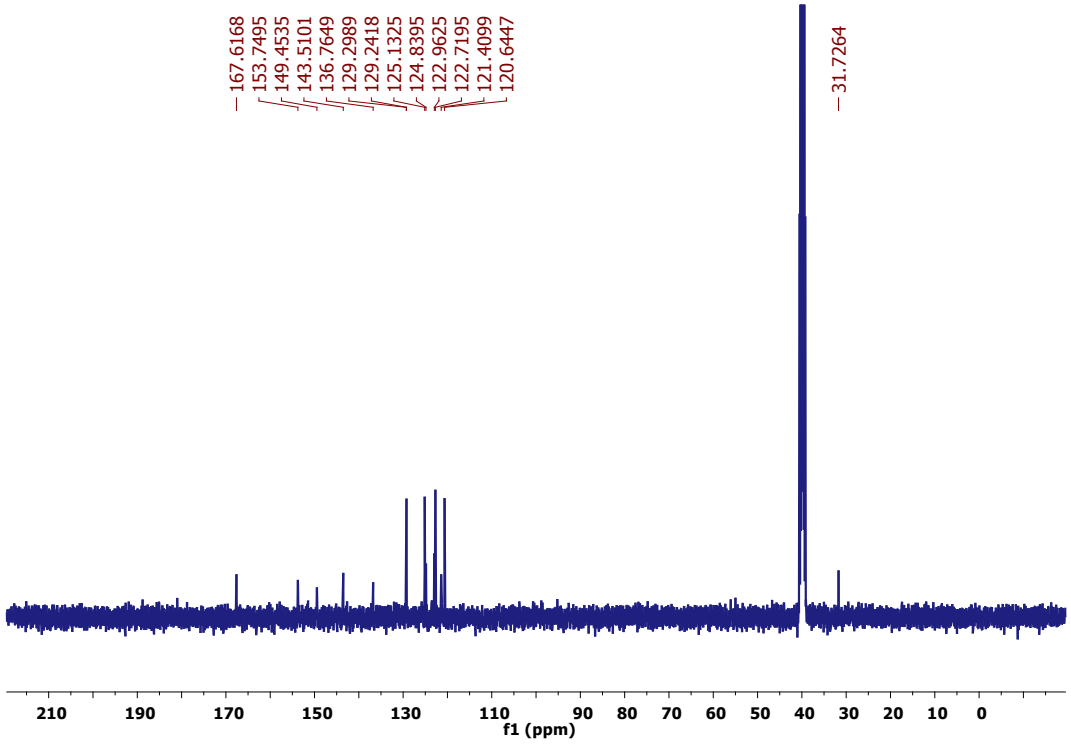
^{1}H NMR spectrum of 4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-pyridin-4-yldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dipyridine (**T3**)in DMSO-d_6



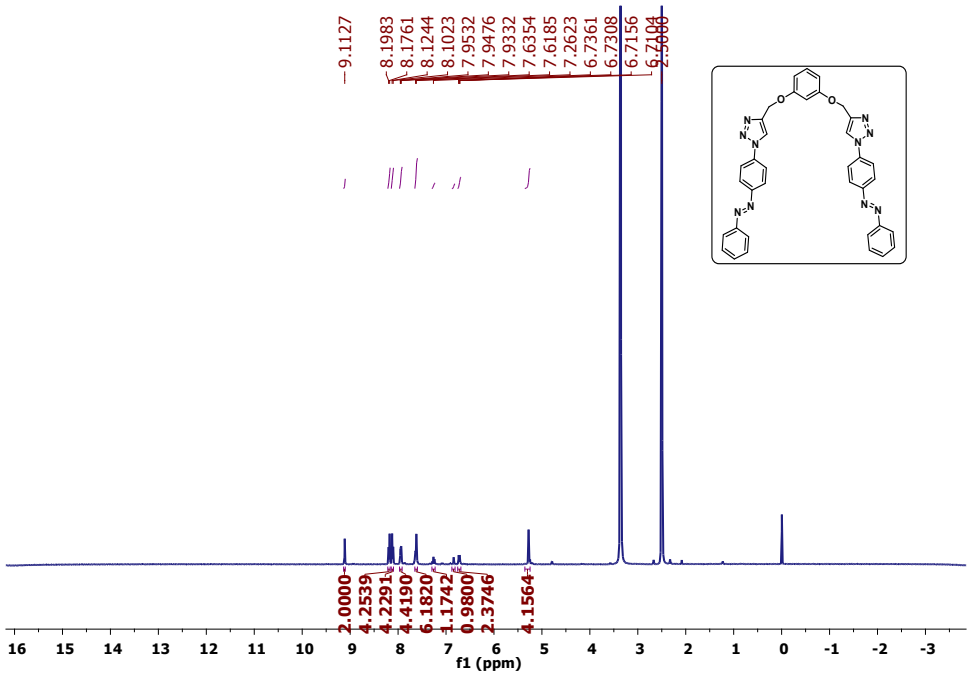
^{1}H NMR spectrum of 3,3'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-pyridin-3-yldiazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dipyridine (**T4**)in DMSO-d_6



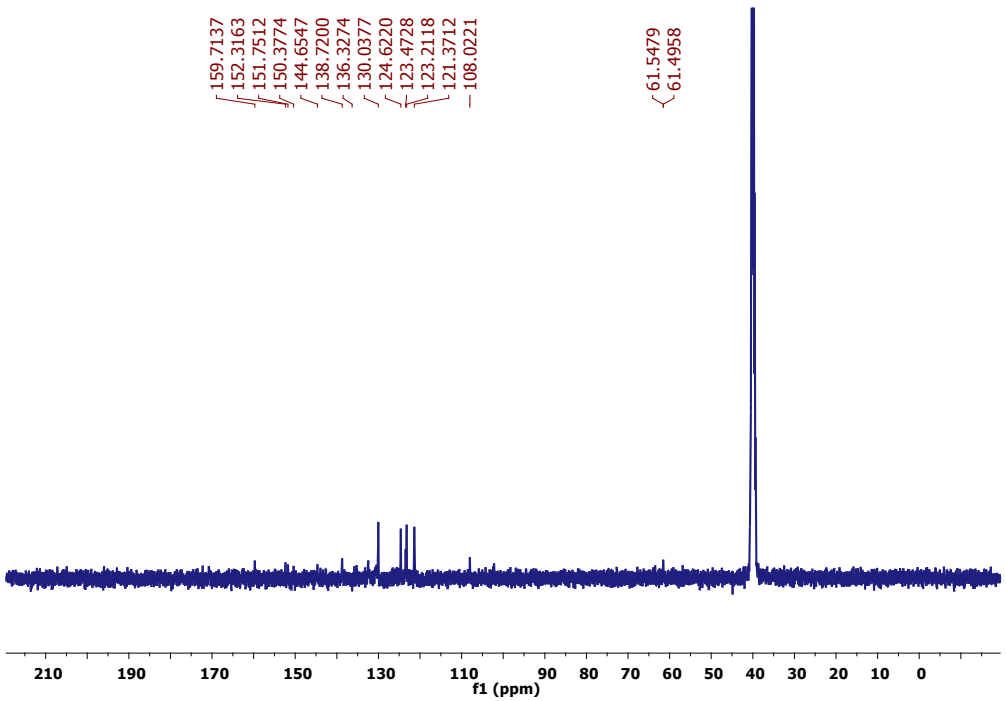
^{1}H NMR spectrum of 4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-(4-carbamoylphenyl)diazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dibenzamide (**T5**) in DMSO-d_6



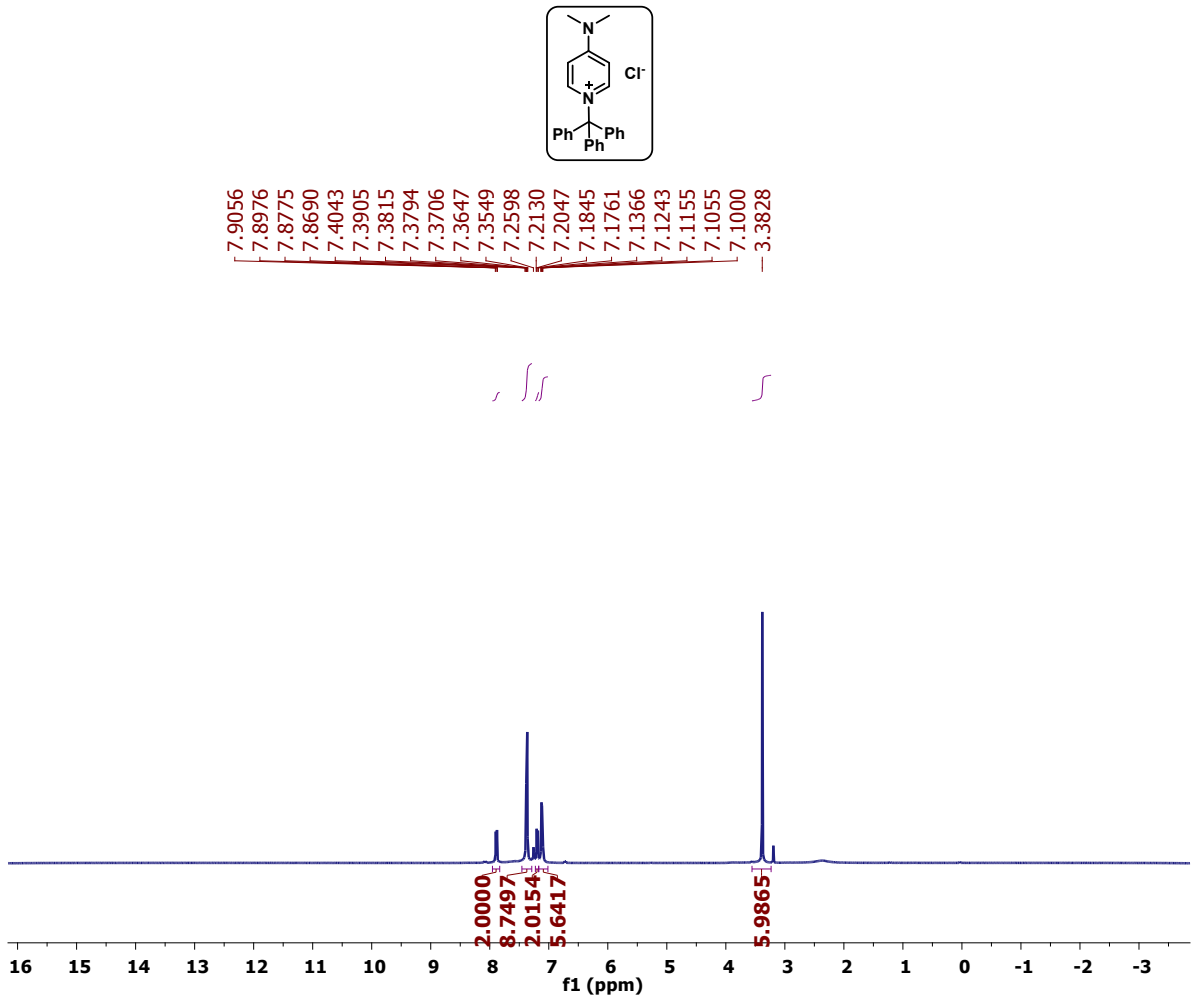
^{13}C NMR spectrum of 4,4'-((1*E*,1'*E*)-(((((5-((2-(4-((*E*)-(4-carbamoylphenyl)diazenyl)phenyl)-2*H*-1,2,3-triazol-4-yl)methoxy)-1,3-phenylene)bis(oxy))bis(methylene))bis(1*H*-1,2,3-triazole-4,1-diyl))bis(4,1-phenylene))bis(diazene-2,1-diyl))dibenzamide (**T5**) in DMSO-d_6



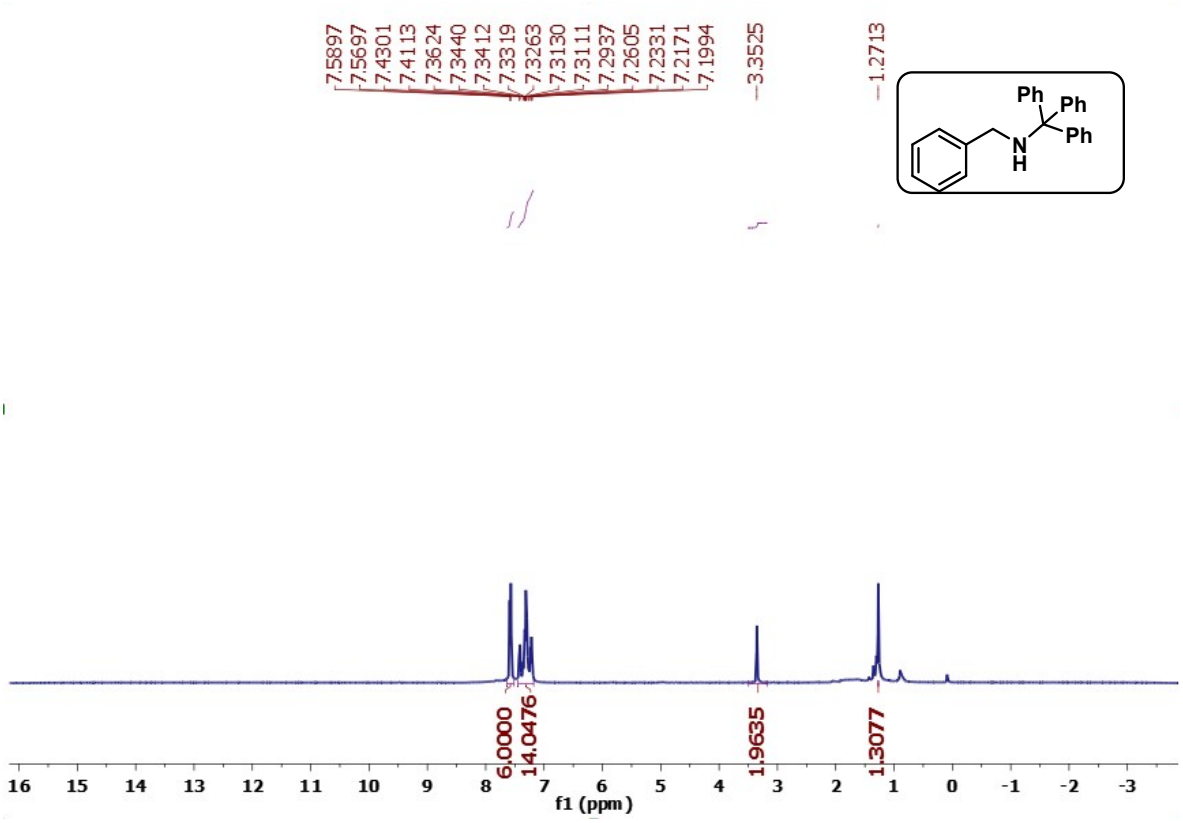
^{1}H NMR spectrum of 1,3-bis((1-(4-((*E*)-phenyldiazenyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzene (**B1**) in DMSO-d_6



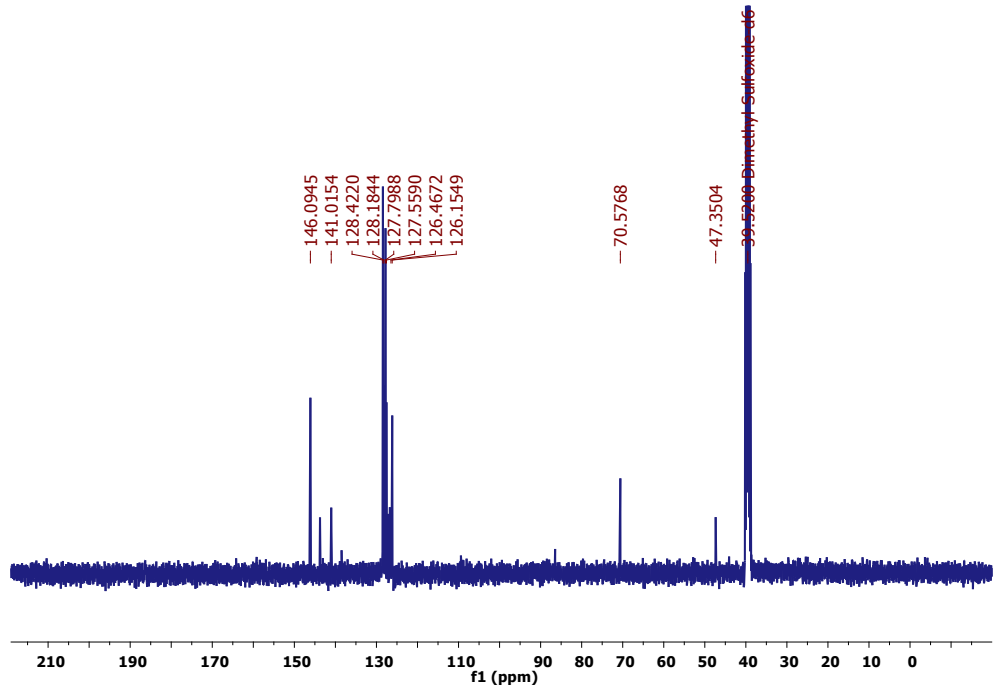
^{13}C NMR spectrum of 1,3-bis((1-(4-((*E*)-phenyldiazenyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzene (**B1**) in DMSO-d_6



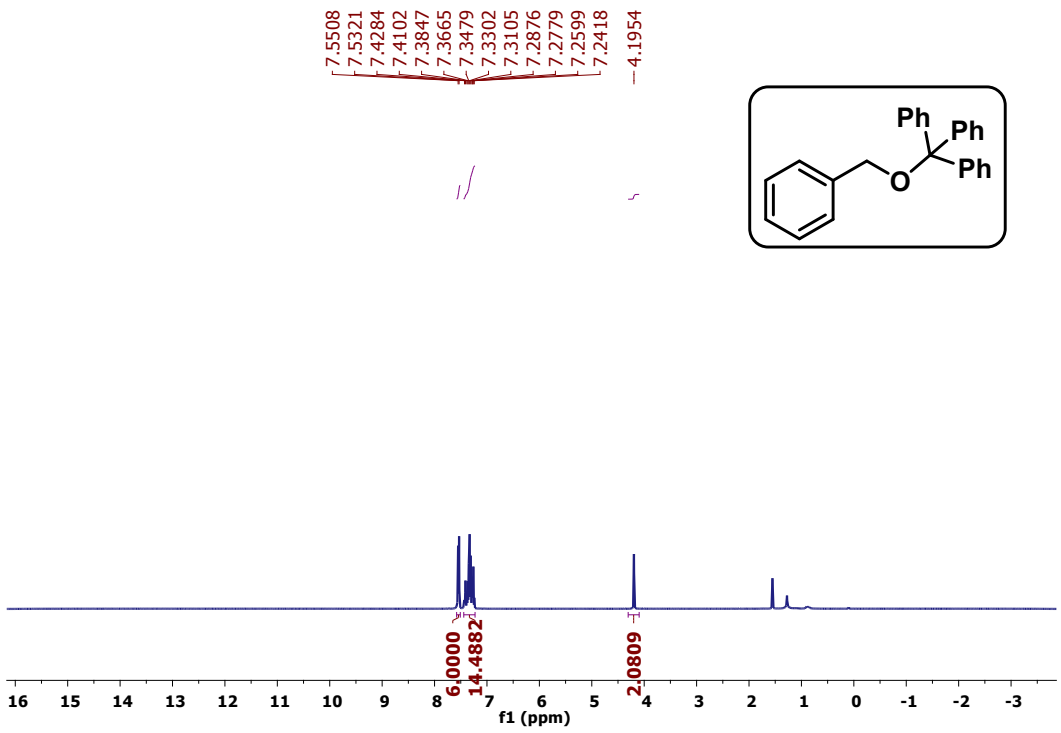
^{1}H NMR spectrum of 4-(dimethylamino)-1-tritylpyridin-1-ium chloride (**A1**) in $CDCl_3$



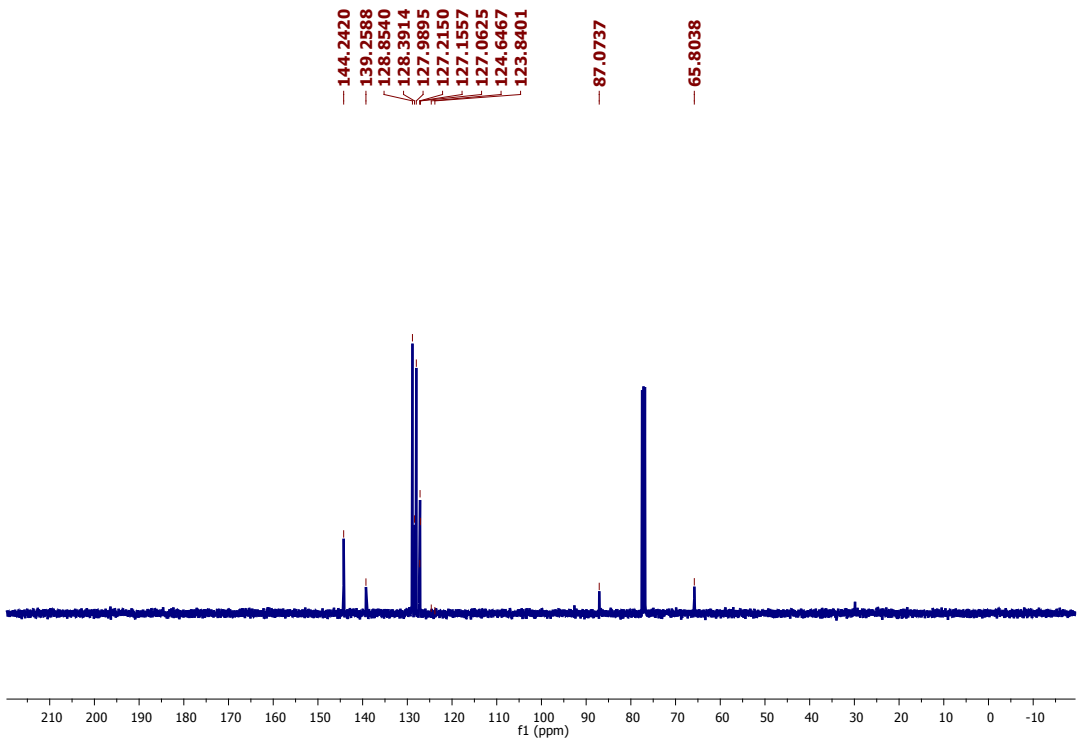
^{1}H NMR spectrum of *N*-benzyl-1,1,1-triphenylmethanamine (**P1**)in $CDCl_3$



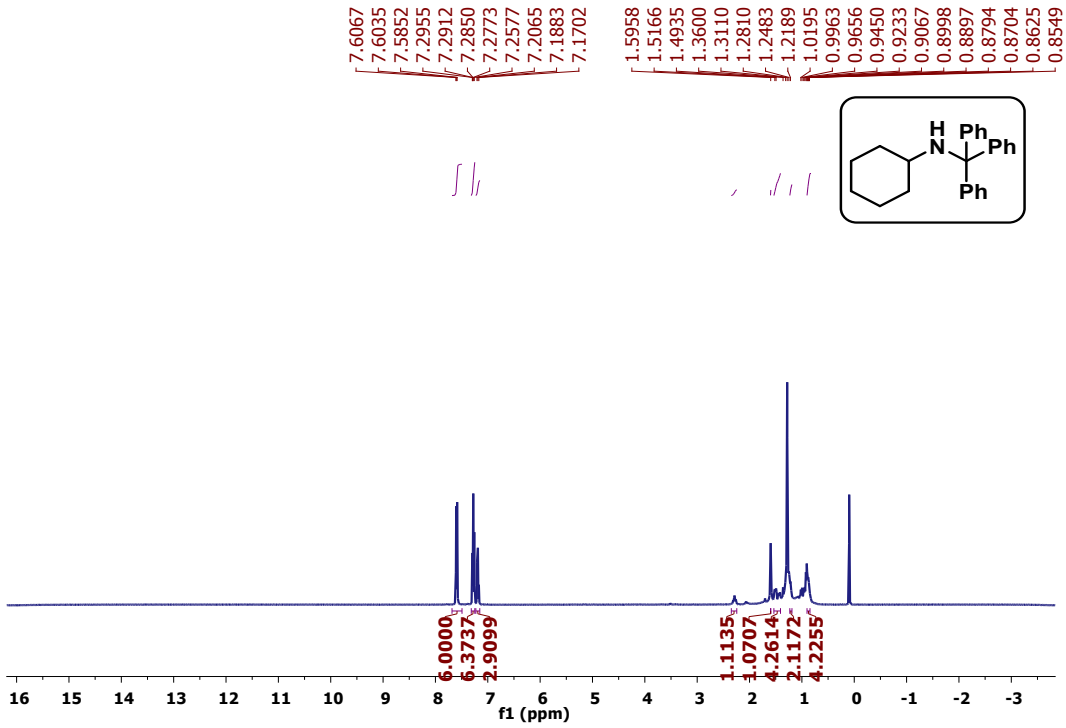
^{13}C NMR spectrum of *N*-benzyl-1,1,1-triphenylmethanamine (**P1**) in DMSO-d_6



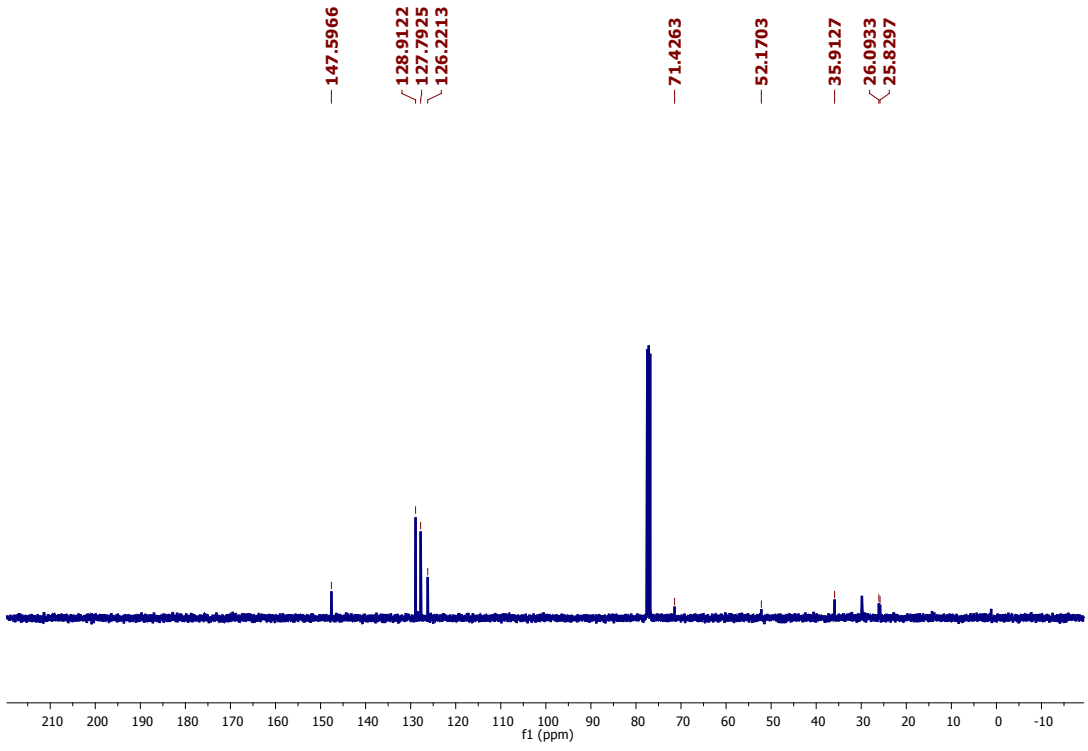
^{1}H NMR spectrum of ((benzyloxy)methanetriyl)tribenzene (**P2**) in $CDCl_3$



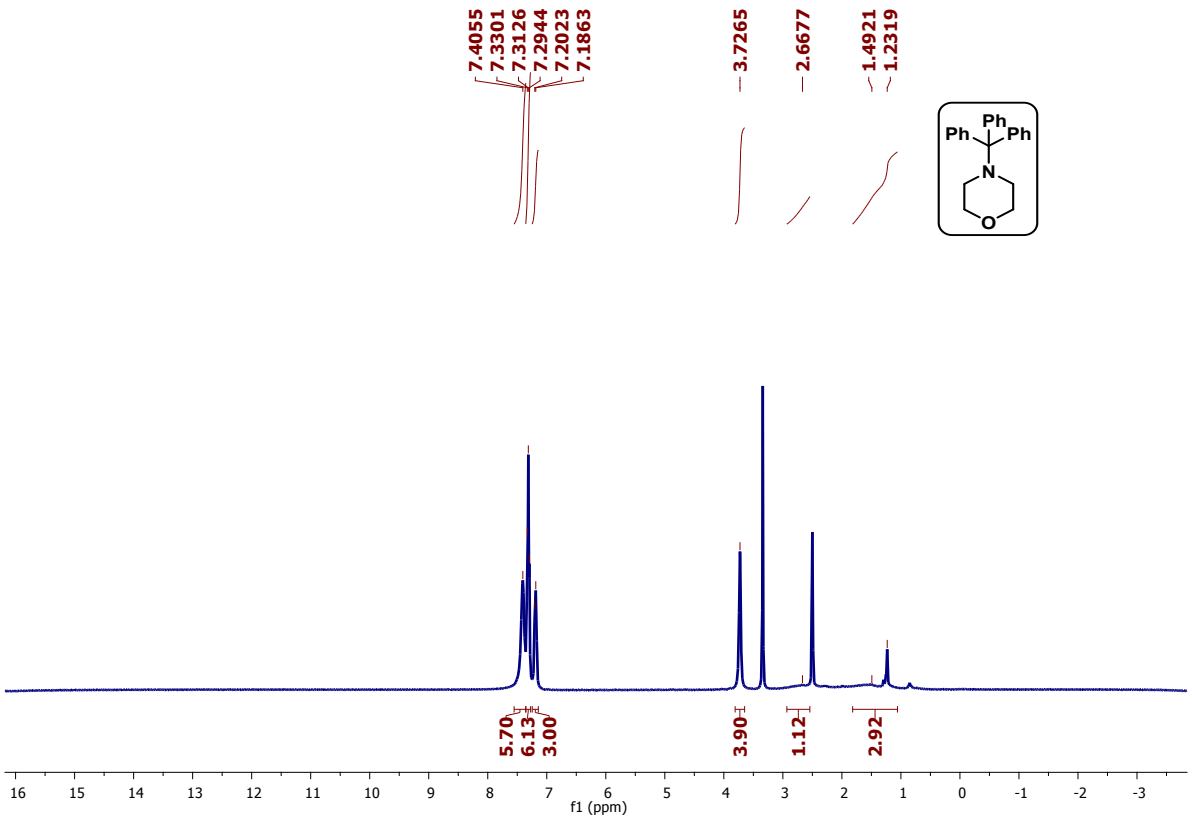
^{13}C NMR spectrum of ((benzyloxy)methanetriyl)tribenzene (**P2**) in $CDCl_3$



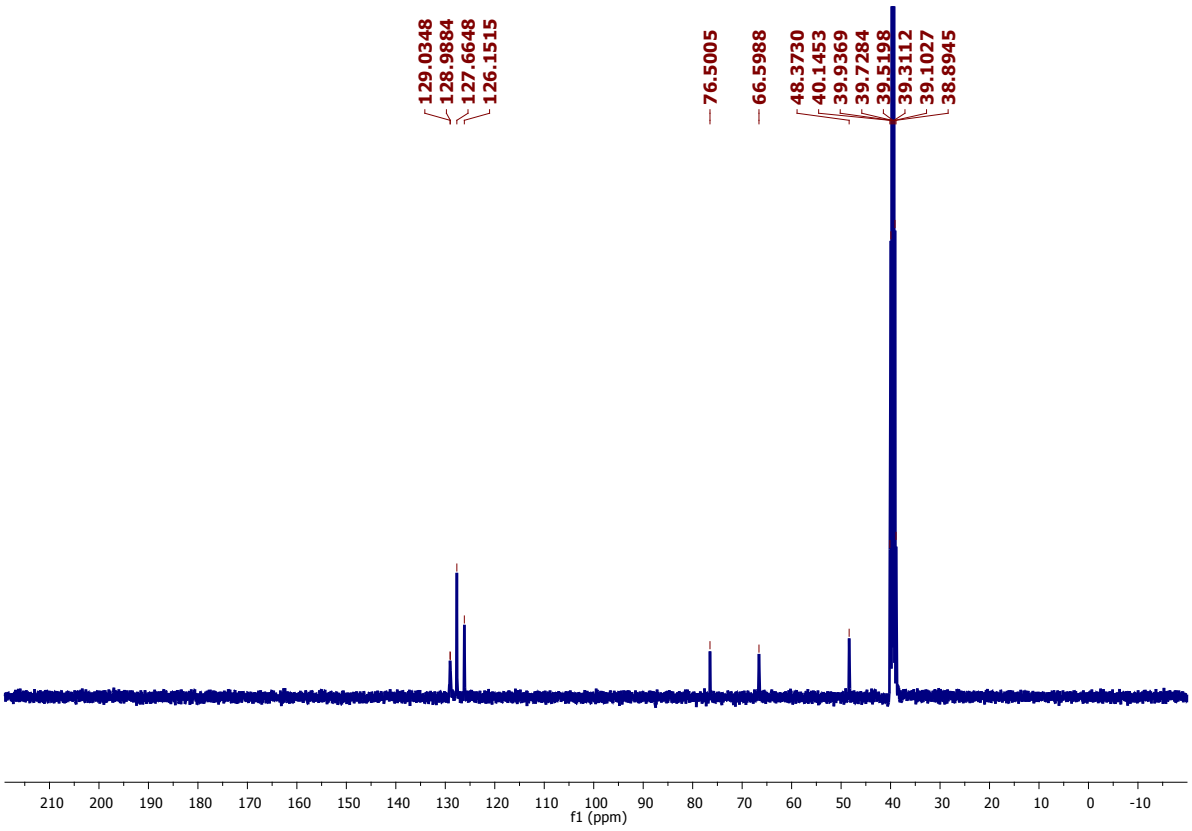
^{1}H NMR spectrum of *N*-Tritylcyclohexanamine(**P3**) in $CDCl_3$



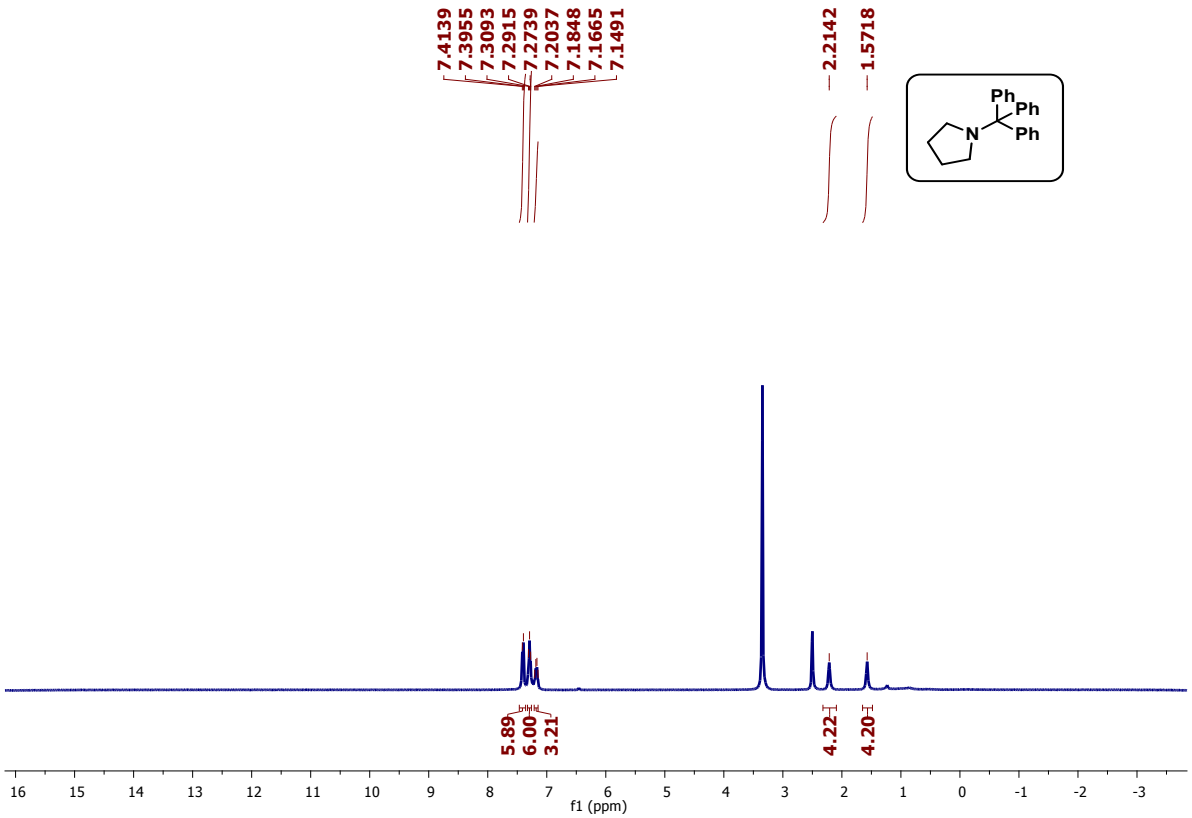
^{13}C NMR spectrum of *N*-Tritylcyclohexanamine(**P3**)in $CDCl_3$



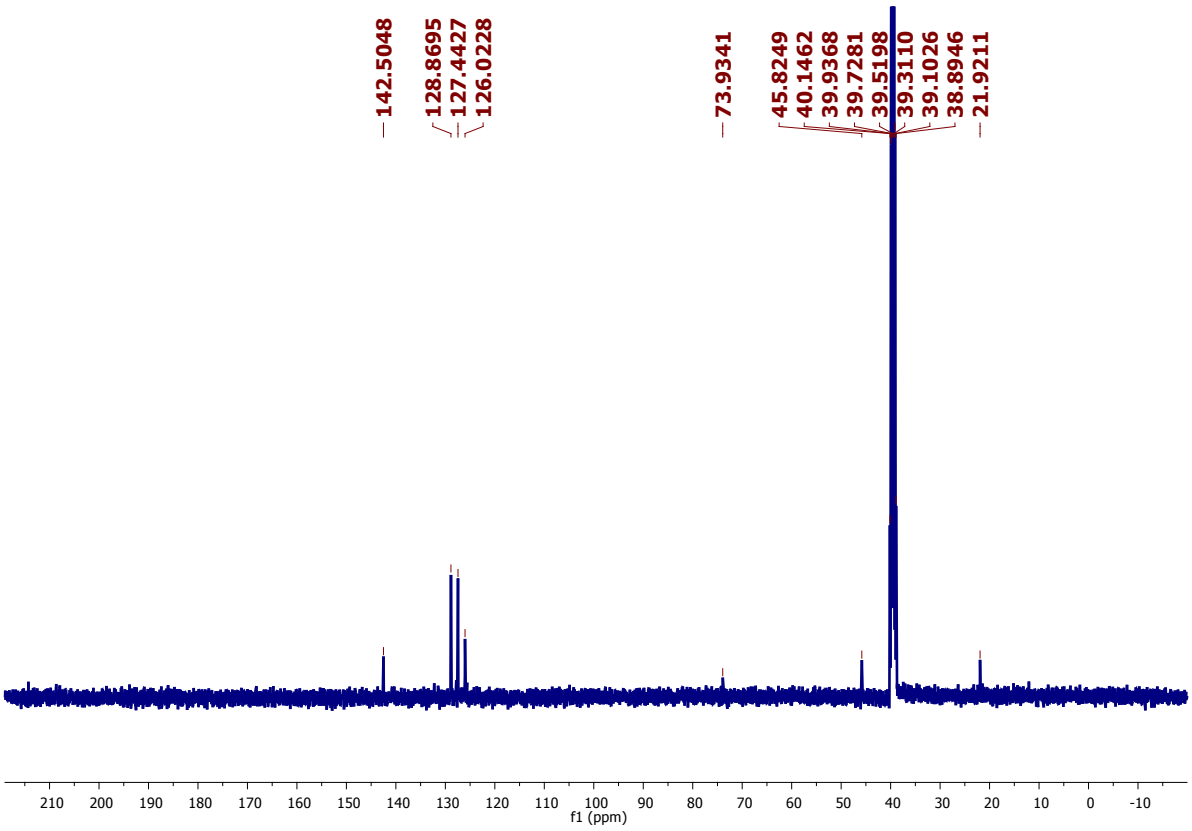
^{1}H NMR spectrum of *N*-Tritylmorpholine(**P4**)in DMSO-d_6



^{13}C NMR spectrum of *N*-Tritylmorpholine (**P4**)in DMSO-d_6.



^{1}H NMR spectrum of *N*-Tritylpyrrolidine (**P5**)in DMSO-d_6



^{13}C NMR spectrum of *N*-Tritylpyrrolidine (**P5**)in DMSO-d_6

S13. Cartesian coordinates

Cartesian coordinates of the optimized structures ofphotoisomers of the catalyst **T1**(*EEE*-, *EEZ*-, *EZZ*- and *ZZZ*-isomers) and their complexes with F^-, Cl^- and Br^-at B3LYP/6-311G(d,p) level of theory:

***EEE*-T1**			
C	-6.26692402	1.01654183	0.51220827
C	-6.07869303	1.42084508	-0.80226566
C	-5.91052004	0.48735127	-1.83698484
C	-5.93786604	-0.86448779	-1.52456009
C	-6.13953503	-1.30461904	-0.20708017
C	-6.29209402	-0.35776923	0.79618801
H	-6.37141701	1.70898367	1.33431340
H	-5.73701405	0.86093946	-2.83515777
H	-6.13437902	-2.36793107	-0.02006738
O	-6.02147503	2.72767615	-1.21060041
O	-6.44994100	-0.65547948	2.12523995
O	-5.75878105	-1.87440061	-2.43324829
C	-5.43780206	-1.54950936	-3.78636723
H	-6.16071106	-0.84872628	-4.21493709
H	-5.53472606	-2.49972626	-4.31406141
C	-6.11152302	3.76976497	-0.24163421
H	-6.98103502	3.64337485	0.41089577
H	-6.26803903	4.67255508	-0.83519204
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H	-7.25721401	-2.57806145	1.96276059
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N	-3.11406100	-3.30985951	2.30241442
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N	-1.95811806	-0.47319534	-3.87394106
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C	-4.87643702	3.88778181	0.59962880
C	-3.56678802	3.63400987	0.27610574
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C	-0.56930906	-0.34603140	-3.60217304
C	0.22727294	0.38922477	-4.48958291
C	-0.01151605	-0.91386461	-2.45542716
C	1.57123494	0.56646572	-4.21823989
H	-0.22993307	0.82537894	-5.36654882
C	1.34179396	-0.73418766	-2.19029913
H	-0.62460804	-1.47113174	-1.75850126
C	2.14172495	0.00833850	-3.06402200
H	2.19971793	1.14109385	-4.88482879
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H	-5.82875704	-1.08760123	2.41058976
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H	-7.30828594	-2.61178681	-1.52964544
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H	0.89537901	4.80340919	3.85083392
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H	5.25545297	1.01419112	-1.06682884
C	8.22250095	1.56712942	-2.64107676
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H	9.25624296	1.81113638	-2.42375572
C	4.42765798	-3.13408023	0.79905538
C	5.07270897	-2.32059405	-0.13873447
C	5.15993599	-4.08557337	1.52572120
C	6.43914497	-2.46797601	-0.36367351
H	4.49272297	-1.59126195	-0.69306132
C	6.52208599	-4.21933933	1.30230616
H	4.64379599	-4.69960051	2.25140309
C	7.16495498	-3.41496015	0.35594731
H	6.93208797	-1.84203587	-1.09793039
H	7.09045499	-4.95123543	1.86523702
H	8.22953198	-3.52803612	0.18403927
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C	5.13227100	0.91560450	2.22559014
C	5.23058301	3.08128329	3.31484655
C	6.46477800	0.68576443	2.55565509
H	4.55148099	0.17925460	1.68350601
C	6.56073601	2.84986923	3.63291550
H	4.73257101	3.99897224	3.59778473
C	7.18071901	1.65345930	3.25786727
H	6.93749300	-0.24545451	2.26612991
H	7.12281402	3.60156613	4.17572263
H	8.21973001	1.48013525	3.51487622

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H	-1.54248297	-1.84255487	-0.63731623
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H	0.72907713	-3.60535642	-4.66574237
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H	-0.52993701	5.64871314	-0.66083239
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H	1.91432999	5.27821711	-0.30185438
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C	4.34030197	-2.56472817	2.42501982
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C	3.27364001	-4.40279105	1.28769360
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C	3.89376999	-5.30188915	2.15447651
H	5.26152996	-5.52613032	3.80270852
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H	3.71791400	-6.36606414	2.04972139
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C	5.62629498	2.42802802	0.71989339
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C	6.95051897	2.24595599	1.09741740
H	4.86831598	1.72161198	1.03182930
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C	7.92459198	3.17823403	0.73061952
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C	4.31712507	-1.39525062	-2.66131906
C	5.04397710	-2.23820352	-3.51693213
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C	7.03929308	-0.95656056	-3.05487195
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O	4.97944823	3.70694877	-0.48899886	O	5.90567805	-0.22475935	-1.20381978
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H	-2.89798340	-9.60743791	2.06781089
H	-1.35372630	-5.95148197	3.70680194
H	-1.84919241	-8.36899195	3.94638792
C	-4.28273282	0.60866115	-2.93492015
C	-3.38889482	0.05320111	-3.85943212
C	-4.91260289	-0.21282083	-1.99314617
C	-3.11484987	-1.31001390	-3.81607112
H	-2.93788577	0.67423109	-4.62196811
C	-4.59848794	-1.56527184	-1.93033016
H	-5.64283789	0.22444020	-1.32297220
C	-3.70440594	-2.12208587	-2.84624013
H	-2.43961887	-1.74187493	-4.54615409
H	-5.07168399	-2.19560482	-1.18629018
H	-3.48031198	-3.18198488	-2.80425813
C	-5.74695688	2.79020821	1.72733480
C	-6.66205691	2.91406825	2.78355877
C	-6.20009584	2.81365123	0.40420179
C	-8.01303889	3.06178930	2.50530373
H	-6.29402694	2.88827923	3.80054278
C	-7.55534082	2.97326928	0.13221474
H	-5.48060082	2.72361620	-0.39947819
C	-8.46343685	3.09429932	1.18182771
H	-8.72341092	3.15038333	3.31959371
H	-7.89570879	3.00033830	-0.89615027
H	-9.52104284	3.21022636	0.97358768

C	0.71235019	1.77016082	-2.66035805
C	0.02772234	3.38573974	-4.82441516
H	1.91300234	2.77580860	-5.67356707
C	-0.50358977	2.44257888	-2.66073413
H	0.98340314	1.14103985	-1.82120201
C	-0.85538870	3.24892784	-3.74808218
H	-0.23386060	4.04996771	-5.63951321
H	-1.17001381	2.35732496	-1.81206415
N	-1.32387388	5.06599930	4.41202170
N	-1.98449466	4.13227389	-3.69414627
N	-5.40936308	-2.63030679	-0.80105302
N	-3.15189069	3.77385096	-3.46082729
N	-2.04386683	5.58379228	3.54101865
N	-6.34358510	-2.55287770	0.01713495
C	-6.21586316	-2.83944163	1.41645897
C	-7.26903321	-3.54800555	2.00317197
C	-5.20319316	-2.29931564	2.21815597
C	-7.26906127	-3.78231248	3.37369298
H	-8.07186421	-3.90782155	1.37051496
C	-5.23333921	-2.50446656	3.59319498
H	-4.41138112	-1.71214870	1.77040496
C	-6.25279627	-3.25944248	4.17276099
H	-8.07368231	-4.35399242	3.82150699
H	-4.45563221	-2.07606657	4.21503798
H	-6.26439131	-3.42339843	5.24388600
C	-3.58635775	2.40822698	-3.42801823
C	-3.23639676	1.46230292	-4.39979217
C	-4.55569780	2.09707108	-2.46760624
C	-3.83576582	0.20687695	-4.38238612
H	-2.52604173	1.71551984	-5.17563816
C	-5.11650186	0.82590811	-2.43114419
H	-4.85436778	2.86293313	-1.76171229
C	-4.76258487	-0.12193096	-3.39253913
H	-3.57903983	-0.51763411	-5.14687907
H	-5.84885590	0.57451919	-1.67306720
H	-5.21733492	-1.10481393	-3.36544709
C	-1.74788578	5.57276619	2.13778966
C	-0.48517575	5.86938111	1.60913269
C	-2.84695376	5.43332720	1.28289263
C	-0.32798970	5.98958603	0.23229269
H	0.35741923	6.03002510	2.26884371
C	-2.67199771	5.51413712	-0.09402936
H	-3.82506178	5.26757927	1.71927061
C	-1.41200668	5.79546303	-0.62392134
H	0.64608232	6.23687396	-0.17422029
H	-3.51686570	5.38640512	-0.76067138
H	-1.28771364	5.87677697	-1.69725334

***EEE*-T1** - F^-			
C	-6.19796599	-0.32918582	1.11587405
C	-6.07162700	1.05060217	1.06275085
C	-5.98689900	1.72684599	-0.16072625
C	-5.98305000	0.98449982	-1.33211314
C	-6.10841800	-0.41027718	-1.31034794
C	-6.18969500	-1.05168000	-0.08366784
H	-6.21023399	-0.88569969	2.04058013
H	-5.83568500	2.79533300	-0.13835541
H	-6.04412300	-0.93860231	-2.24946086
O	-5.98026199	1.85859533	2.16431773
O	-6.22918199	-2.41091097	0.07497336

***ZEE*-T1** - F^-			
C	-5.84203902	-1.23049899	0.84625891
C	-5.94141900	0.09728102	0.45893993
C	-5.84794097	0.47086105	-0.88749706
C	-5.60294896	-0.51124094	-1.83547807
C	-5.49726499	-1.86049095	-1.47495810
C	-5.59394102	-2.19987997	-0.13381911
H	-5.85263905	-1.54710101	1.87814890
H	-5.87868295	1.52389405	-1.12263704
H	-5.25149898	-2.57241693	-2.24818811
O	-6.09580600	1.14492300	1.32716895
O	-5.42220004	-3.46732699	0.35518687

O	-5.82201501	1.51870664	-2.58248322
C	-5.51079701	2.89916162	-2.70911143
H	-6.21512201	3.50537570	-2.12541951
H	-5.67698301	3.13616046	-3.76087646
C	-5.87856599	1.26311652	3.45038582
H	-6.67528199	0.52191154	3.59291493
H	-6.06241799	2.07313063	4.15747770
C	-6.06166100	-3.24489814	-1.06305152
H	-6.73776200	-2.93180326	-1.86880857
H	-6.38103999	-4.23737309	-0.74221538
C	-4.64895200	-3.33946221	-1.56767851
C	-3.54050000	-2.54532718	-1.38299663
N	-2.57501100	-3.16589629	-2.12859654
H	-3.35207500	-1.63008910	-0.82133877
C	-4.09305301	3.25480967	-2.35860348
C	-3.12039301	2.59644978	-1.64225139
N	-2.05911301	3.45991378	-1.67611952
H	-3.08195700	1.63874086	-1.12257325
C	-4.53652199	0.65942457	3.75670990
C	-3.48776299	0.26816445	2.95634995
N	-2.56938099	-0.21728941	3.84721002
H	-3.31468499	0.27870130	1.88063995
N	-4.31746400	-4.38072333	-2.38928136
N	-3.07372400	-4.27878238	-2.73135938
N	-4.21761698	0.40579576	5.06156094
N	-3.03812598	-0.12353523	5.12036901
N	-3.59412901	4.45323361	-2.78822366
N	-2.37374501	4.58207167	-2.37832668
C	-0.77310701	3.32662086	-1.08974750
C	0.19687499	4.30924683	-1.35095765
C	-0.48627900	2.23537299	-0.26639534
C	1.45516399	4.19812491	-0.79256164
H	-0.06114501	5.14091773	-1.99065577
C	0.78584200	2.13663107	0.28516567
H	-1.23553800	1.46630101	-0.06721323
C	1.76516200	3.10366203	0.03197952
H	2.21608799	4.94235388	-0.98532675
H	1.04003300	1.30128816	0.92629679
C	-1.28572899	-0.77426345	3.60324710
C	-0.47627898	-1.11727729	4.69126015
C	-0.84850199	-0.97974664	2.28664813
C	0.77652502	-1.66199632	4.45835422
H	-0.84235798	-0.95311814	5.69414713
C	0.41084201	-1.51782267	2.07172720
H	-1.48140099	-0.71160077	1.43796009
C	1.23929701	-1.85899251	3.15258925
H	1.42571802	-1.93570620	5.28154826
H	0.76744301	-1.68457182	1.06408723
C	-1.22382500	-2.78738732	-2.34730960
C	-0.39045200	-3.63856143	-3.08067248
C	-0.74489200	-1.56955225	-1.84221178
C	0.92485500	-3.26727346	-3.30915854
H	-0.78751800	-4.56901448	-3.45921834
C	0.57397400	-1.21454128	-2.07785484
H	-1.39434200	-0.91193316	-1.26085688
C	1.42381300	-2.05836739	-2.81093272
H	1.59317400	-3.90729654	-3.87284345
H	0.96135100	-0.27752722	-1.70107098
N	2.53738501	-2.40306153	3.03685433
N	2.77933700	-1.78980143	-3.10024776

O	-5.40702993	-0.26435391	-3.16796406
C	-5.31028491	1.08148410	-3.61434403
H	-6.15806891	1.66985110	-3.24111204
H	-5.40595789	1.03182412	-4.69978304
C	-6.03362203	0.89994397	2.72565395
H	-6.70368305	0.07481697	2.99861792
H	-6.42798903	1.80288797	3.19373196
C	-4.99137504	-4.49693697	-0.52452314
H	-5.62084202	-4.52132195	-1.42313216
H	-5.16610306	-5.42815498	0.01610583
C	-3.53796103	-4.42917198	-0.90136211
C	-2.61269702	-3.41293399	-0.84539608
N	-1.47792201	-3.98496500	-1.35302406
H	-2.65017901	-2.37530000	-0.51392005
C	-4.01038991	1.75913907	-3.28157199
C	-3.03106793	1.48452804	-2.35403998
N	-2.12043391	2.48678304	-2.54491694
H	-2.90127495	0.70863802	-1.59968299
C	-4.65006005	0.65298194	3.25850297
C	-3.47622204	0.26745994	2.65273699
N	-2.58960806	0.19193691	3.69233600
H	-3.19577002	0.04472196	1.62285299
N	-2.94186103	-5.54461998	-1.42117513
N	-1.70506902	-5.28161999	-1.69668210
N	-4.43075507	0.79751191	4.60008598
N	-3.19508208	0.51810389	4.86571900
N	-3.65974588	2.88094908	-3.97840696
N	-2.52581788	3.32363106	-3.53634193
C	-0.90432592	2.74260301	-1.85441891
C	-0.54562895	1.96935198	-0.74618692
C	-0.06956490	3.77006601	-2.30931387
C	0.65899704	2.23664995	-0.10554489
H	-1.17888297	1.14765398	-0.40391295
C	1.10508309	4.05592098	-1.63213085
H	-0.35911988	4.33459203	-3.18385187
C	1.47173006	3.30031695	-0.51093285
H	0.97607801	1.62590893	0.73170210
H	1.74755411	4.85036298	-1.98925982
C	-1.22283607	-0.19596611	3.68268402
C	-0.49054309	-0.13687214	4.87278104
C	-0.62934605	-0.64590509	2.49412202
C	0.83790591	-0.53241016	4.87143405
H	-0.97456110	0.21009285	5.77399303
C	0.70151095	-1.03379110	2.50958604
H	-1.20067203	-0.68408206	1.56493601
C	1.45021392	-0.98078114	3.69583706
H	1.42897289	-0.49863818	5.77889907
H	1.17684996	-1.38841809	1.60478304
C	-0.19904700	-3.40584001	-1.56437203
C	0.85338600	-4.22393301	-2.00857202
C	-0.00207099	-2.04175102	-1.33769000
C	2.10381501	-3.67763402	-2.22353799
H	0.66395099	-5.27455401	-2.17559405
C	1.26220202	-1.50798903	-1.55707096
H	-0.81504099	-1.40679601	-0.98088000
C	2.32232302	-2.30842203	-1.99666596
H	2.92773901	-4.29143102	-2.56187799
H	1.44764603	-0.45391703	-1.39010893
N	2.80703192	-1.35557716	3.81480207
N	3.55693503	-1.65022704	-2.16764992

N	3.01866200	2.88205512	0.63712655
N	3.23638000	-0.72934635	-2.60669392
N	2.98771401	-2.47062570	1.86705134
N	3.89193200	3.76068309	0.42668342
C	5.14749600	3.50652719	1.03850245
C	6.11875000	4.49773416	0.86146931
C	5.45853700	2.35334729	1.77564262
C	7.38614700	4.34773624	1.41660532
H	5.85145899	5.37668808	0.28665318
C	6.72509801	2.20885338	2.32436464
H	4.69896701	1.59326231	1.90104874
C	7.69251500	3.20267835	2.14915349
H	8.13276800	5.12188422	1.27733021
H	6.96416801	1.31481146	2.88969477
H	8.67982000	3.08064842	2.58110351
C	4.59500799	-0.46003040	-2.91200996
C	5.14738499	0.65419570	-2.27158413
C	5.38118299	-1.21851252	-3.79325685
C	6.47514299	1.00518467	-2.49710818
H	4.51867800	1.22466080	-1.59875921
C	6.70276299	-0.85917155	-4.01792791
H	4.93367699	-2.07227660	-4.28473673
C	7.25518299	0.25057054	-3.37053507
H	6.89696599	1.86489574	-1.98942531
H	7.30983099	-1.44220365	-4.70263583
H	8.28913599	0.52409452	-3.55095012
C	4.28622301	-3.02893771	1.75398042
C	4.85266501	-2.98247990	0.47603441
C	5.00086402	-3.60955355	2.81285250
C	6.12586501	-3.49929093	0.25528448
H	4.27820301	-2.53132002	-0.32364666
C	6.26704202	-4.12916159	2.58424057
H	4.54286502	-3.63969241	3.79262950
C	6.83489501	-4.07469177	1.30750056
H	6.56091401	-3.45034207	-0.73632953
H	6.81869402	-4.58166947	3.40162764
H	7.82573401	-4.48186780	1.13720562
F	-2.58412800	0.04243002	-0.00646002

N	2.73264405	3.43572892	0.15166917
N	4.50688703	-2.36301404	-2.57738691
N	3.36667493	-1.69210914	2.74300108
N	3.24302605	4.52753991	0.46530721
C	2.55599607	5.78663392	0.39896122
C	3.26877809	6.87005692	-0.12402974
C	1.31126506	6.00043192	1.00341220
C	2.71187811	8.14433793	-0.10820873
H	4.25379810	6.69193192	-0.54009873
C	0.77738507	7.28382393	1.04620822
H	0.77324804	5.16855492	1.44022617
C	1.46457510	8.35650293	0.47818825
H	3.25944713	8.97577893	-0.53849070
H	-0.18494293	7.44447293	1.51932020
H	1.03689111	9.35228093	0.50560726
C	5.74040404	-1.67584805	-2.72538288
C	5.95912405	-0.33980707	-2.35512084
C	6.78905204	-2.42385306	-3.27116387
C	7.21221206	0.22774192	-2.53909481
H	5.14141205	0.22501294	-1.92747285
C	8.04200205	-1.84706207	-3.45666483
H	6.59259804	-3.45406105	-3.54412790
C	8.25672106	-0.51982308	-3.09081080
H	7.38025707	1.25867092	-2.24735478
H	8.84890106	-2.43219707	-3.88406883
H	9.23269607	-0.06780509	-3.23019677
C	4.72535593	-2.07781016	2.87025310
C	5.40820490	-2.20240319	4.08967011
C	5.39084795	-2.35109514	1.67083510
C	6.73939690	-2.59318621	4.09585312
H	4.87497189	-1.98857621	5.00641210
C	6.72787694	-2.73733816	1.68366512
H	4.84148197	-2.24773612	0.74306709
C	7.40441492	-2.86066019	2.89522913
H	7.26683288	-2.69172824	5.03885913
H	7.23775796	-2.93976015	0.74880413
H	8.44557391	-3.16456221	2.90818915
F	-2.27301700	-0.44782101	-0.08116101

***ZZE*-T1** - F^-

C	-5.39604103	-0.68823898	1.58938305
C	-5.33519201	0.66465704	1.29072812
C	-5.36834901	1.11948211	-0.03338686
C	-5.40190104	0.18461716	-1.05699791
C	-5.46201506	-1.18834385	-0.78702398
C	-5.43934305	-1.60864792	0.53423000
H	-5.32152102	-1.07518103	2.59436003
H	-5.26452600	2.17980511	-0.20603280
H	-5.43362208	-1.86949681	-1.62382701
O	-5.19945198	1.65597599	2.22578117
O	-5.42094707	-2.92043794	0.92553993
O	-5.33774505	0.49712423	-2.38847889
C	-5.14529603	1.85119825	-2.77336982
H	-5.87664101	2.49823623	-2.27215978
H	-5.36777504	1.87978130	-3.84108882
C	-4.95674698	1.30055491	3.58014315
H	-5.69525599	0.56377591	3.92068912
H	-5.12737196	2.21384089	4.15168420
C	-5.26714009	-3.93389089	-0.05995812
H	-5.98046710	-3.78062484	-0.87945611

***ZZZ*-T1** - F^-

C	2.30217419	-4.52148883	0.74101942
C	1.04188921	-4.88334493	0.28926846
C	0.69616919	-4.77785106	-1.06387855
C	1.62292016	-4.24587310	-1.94777560
C	2.90673515	-3.88068200	-1.52329264
C	3.22050816	-3.99654287	-0.17718563
H	2.58153620	-4.53469473	1.78359242
H	-0.31671480	-5.02020213	-1.34703852
H	3.56751012	-3.42486403	-2.24475268
O	0.02878323	-5.32241890	1.09928150
O	4.40006015	-3.57909977	0.37849932
O	1.36749114	-3.98569622	-3.26795062
C	0.05054915	-4.17017133	-3.76908860
H	-0.31213780	-5.17698432	-3.52450451
H	0.14802014	-4.11745342	-4.85434560
C	0.20110924	-5.27450177	2.50945650
H	1.14346626	-5.75873571	2.79542553
H	-0.60838873	-5.88012178	2.91876656
C	5.35214311	-2.90927179	-0.43691974
H	5.55197013	-3.49408686	-1.34427769

H	-5.54314210	-4.86443991	0.43743483
C	-3.86839410	-4.07886689	-0.59008414
C	-2.79570509	-3.21650990	-0.62661311
N	-1.81996910	-3.94641788	-1.24641815
H	-2.63615007	-2.19334092	-0.28847306
C	-3.75232802	2.37286421	-2.55585681
C	-2.69780902	1.90725916	-1.80420984
N	-1.72614901	2.84904815	-2.00032880
H	-2.55440303	1.03732112	-1.16229989
C	-3.56196398	0.81597388	3.86311311
C	-2.56656100	0.31633590	3.05447407
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C	0.62567800	-0.68126023	4.73726699
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C	-4.70909103	-2.46518039	-2.54447357	C	6.71618097	-1.09472532	-2.85836593
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C	-5.45482204	-2.93235657	-3.63729949	C	7.91170095	-1.68106838	-3.28627491

C	-6.73627902	-2.30586119	-1.23082858	C	7.86171606	1.01396564	-2.59165798
H	-4.75849902	-1.79661107	-0.51455968	H	5.76120405	0.70731274	-2.19282998
C	-6.82942304	-3.08054855	-3.51862446	C	9.07822298	-0.92601743	-3.36134692
H	-4.93538305	-3.16763571	-4.55677246	H	7.89817391	-2.73154238	-3.55176489
C	-7.47491203	-2.76947136	-2.31771550	C	9.05659904	0.42317158	-3.01405096
H	-7.22820501	-2.06561404	-0.29515261	H	7.84254911	2.06537365	-2.32624301
H	-7.40655205	-3.43992969	-4.36409340	H	10.00154597	-1.38888348	-3.69169091
H	-8.54956703	-2.88958435	-2.23319047	H	9.96289707	1.01568554	-3.07452497
C	-4.53503804	3.92637683	-1.15964659	C	5.50422598	-0.19658911	3.09103804
C	-5.23587704	2.75916377	-1.48152540	C	6.23683298	0.00909589	4.26991304
C	-5.21038604	5.15578383	-1.12553778	C	6.16276299	-0.20610617	1.85688004
C	-6.59723804	2.81360173	-1.76696839	C	7.60942199	0.20017683	4.20164204
H	-4.69073103	1.82315077	-1.50411025	H	5.70871898	0.01550993	5.21417903
C	-6.56757504	5.20351478	-1.41034777	C	7.54022300	-0.01663423	1.79522804
H	-4.65132404	6.04733387	-0.87438792	H	5.57429898	-0.36746517	0.96153404
C	-7.26604904	4.03550073	-1.73156658	C	8.26582600	0.18770077	2.96693104
H	-7.13088204	1.90400368	-2.01828124	H	8.17602699	0.36177282	5.11262304
H	-7.08959304	6.15417178	-1.38358292	H	8.04185800	-0.02735928	0.83435205
H	-8.32654004	4.08185769	-1.95421958	H	9.33897800	0.33867672	2.92227104
Cl	2.36923598	0.11153002	-0.01273705	Cl	-1.70394103	-0.76264988	-0.18304699
***ZZE*-T1** - Cl^-				***ZZZ*-T1** - Cl^-			
C	-5.33609311	-1.37736054	1.28484412	C	3.47994154	-3.98906735	0.65318288
C	-5.31099099	-0.02323754	1.58214709	C	2.26700648	-4.65390523	0.74719486
C	-5.42103792	0.94504345	0.57467308	C	1.50688044	-4.94621212	-0.39363215
C	-5.52780397	0.52600444	-0.74239292	C	1.97765648	-4.53511613	-1.63084414
C	-5.54153509	-0.83585057	-1.07474689	C	3.19800255	-3.85701725	-1.75729912
C	-5.44310116	-1.77191556	-0.05663087	C	3.93041858	-3.58628336	-0.61174711
H	-5.21232117	-2.14808354	2.03087313	H	4.06793158	-3.70852344	1.51422088
H	-5.35026782	1.98392145	0.86010705	H	0.54973739	-5.42623402	-0.25544816
H	-5.58170812	-1.09883959	-2.12101688	H	3.49233259	-3.52166825	-2.74043211
O	-5.16403593	0.49045547	2.84380108	O	1.69884143	-5.06618021	1.92311485
O	-5.43952828	-3.12961256	-0.24361785	O	5.12279165	-2.91093349	-0.59640209
O	-5.61751291	1.37002142	-1.81831893	O	1.31390046	-4.73000502	-2.81363514
C	-5.68917778	2.77435943	-1.60780896	C	0.09552339	-5.46134890	-2.82030216
H	-6.31653675	2.99879750	-0.73737095	H	0.16663530	-6.33047692	-2.15566619
H	-6.19573776	3.17862046	-2.48597096	H	-0.01299266	-5.83981285	-3.83827017
C	-5.07743399	-0.38822451	3.95741010	C	2.39652646	-4.87577832	3.14640385
H	-5.80520007	-1.20274445	3.86080512	H	3.46236043	-5.09934242	3.01960684
H	-5.37248393	0.20836153	4.82250709	H	1.98943438	-5.62032329	3.83300983
C	-5.42131534	-3.66982559	-1.56036984	C	5.68812070	-2.45235851	-1.81728108
H	-6.05501730	-3.07959155	-2.23068884	H	5.57909362	-3.21016547	-2.60181210
H	-5.87251942	-4.65998255	-1.47958481	H	6.75610171	-2.34216763	-1.62097108
C	-4.03693536	-3.84122072	-2.11506785	C	5.15415984	-1.12422244	-2.27036304
C	-2.86058330	-3.18104182	-1.85144187	C	4.02412691	-0.42723133	-1.91652302
N	-1.93981737	-3.82789791	-2.62635387	N	4.11421503	0.73056568	-2.63676898
H	-2.61769222	-2.34485582	-1.20870089	H	3.20263789	-0.65364727	-1.24985402
C	-4.34844072	3.44028032	-1.49653698	C	-1.11440853	-4.63368978	-2.49581614
C	-3.10819476	2.94332222	-1.17666099	C	-1.24728040	-3.40677378	-1.89139310
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H	-2.76605284	1.95459919	-0.89597097	H	-0.52939733	-2.72108287	-1.45944908
C	-3.69949904	-0.93223463	4.20510309	C	2.20352460	-3.51709931	3.75611389
C	-2.58524105	-0.99792674	3.40492008	C	1.73279172	-2.33601525	3.23386793
N	-1.64539810	-1.59467281	4.19891008	N	1.77342781	-1.47144529	4.29149095
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N	-2.53123846	-4.82772287	-3.33169185	N	5.24279303	0.73271058	-3.39324398
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C	-0.23934156	5.34594397	-1.29943807
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C	1.13003246	5.45262285	-1.11605608
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C	1.87955736	4.32931979	-0.74121407
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C	-0.29818013	-1.93835793	3.90298707
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C	0.21291287	-1.73766300	2.61391906
C	1.81452180	-2.83195210	4.62032207
H	0.08837383	-2.62788592	5.89719608
C	1.52144084	-2.09650312	2.33709406
H	-0.39497410	-1.30334096	1.82512106
C	2.33665780	-2.65144117	3.33438906
H	2.45797277	-3.25655214	5.38172407
H	1.92591984	-1.95557917	1.34425305
C	-0.53480935	-3.62444203	-2.71804289
C	0.24934156	-4.56128312	-3.40061588
C	0.05854375	-2.52271707	-2.09751292
C	1.62479058	-4.39641124	-3.44228490
H	-0.22753252	-5.41595508	-3.85830486
C	1.43359577	-2.34954619	-2.17721394
H	-0.52811018	-1.79531801	-1.54262493
C	2.23103268	-3.27712428	-2.85915793
H	2.25492751	-5.13832830	-3.91855189
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C	3.97722765	7.53887564	0.47980084
C	2.61005454	6.00257478	1.75802989
C	3.59168175	8.57950769	1.31802183
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C	2.25872564	7.04172183	2.61265787
H	2.23720045	5.00113481	1.93183391
C	2.73248774	8.33431778	2.38858284
H	3.97646884	9.57879065	1.14659580
H	1.60528363	6.84105390	3.45424188
H	2.44526082	9.14119482	3.05309683
C	3.89268087	-0.97242643	-3.27995799
C	3.16221088	-0.75001539	-4.45241699
C	4.31692498	0.11039555	-2.50410902
C	2.83012299	0.55013363	-4.81780301
H	2.86079880	-1.58914237	-5.06741897
C	3.94494509	1.40504757	-2.85337104
H	4.91689997	-0.08041449	-1.62166302
C	3.20246609	1.62658762	-4.01354503
H	2.26367699	0.72114367	-5.72662301
H	4.22501017	2.24136056	-2.22253906
H	2.91870518	2.63562264	-4.28883405
C	5.45891773	-3.35829547	1.79447704

N	-3.24496448	-4.21423456	-2.50052112
C	-3.32674726	-2.04443758	-1.45903405
C	-2.67273314	-0.97720167	-0.83881302
C	-4.71012125	-2.00328943	-1.67099605
C	-3.40978003	0.13690140	-0.45881899
H	-1.60035914	-0.98646278	-0.65893202
C	-5.44230714	-0.90719837	-1.24319402
H	-5.19010434	-2.83266536	-2.16996307
C	-4.79684302	0.17108255	-0.62438898
H	-2.90613194	0.98800933	-0.01716096
H	-6.51107413	-0.87796525	-1.41296601
C	1.39189596	-0.10213325	4.36243100
C	1.34659402	0.52360072	5.61348702
C	1.04698803	0.60206082	3.20598602
C	0.95589116	1.84995976	5.69987906
H	1.59922997	-0.04499933	6.49666000
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H	1.04664698	0.12717385	2.22810000
C	0.66306124	2.58490782	4.54558008
H	0.87207821	2.33912774	6.66328907
H	0.42938622	2.47896091	2.40029508
C	3.24800815	1.85855677	-2.64526695
C	3.66445927	3.03393675	-3.28082191
C	2.01244214	1.80302388	-1.99669895
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H	4.62997727	3.05845966	-3.76518691
C	1.18744626	2.91978097	-2.00028391
H	1.67803505	0.90769290	-1.47897097
C	1.58967938	4.10117094	-2.63414588
H	3.17238848	5.08639281	-3.69108785
H	0.23938726	2.86699205	-1.48264191
N	0.16024238	3.91007587	4.75700912
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N	0.44526848	4.89533986	4.05064715
N	-6.55406789	1.48073170	0.27099306
C	-7.19161600	0.37216675	0.92328003
C	-8.57547601	0.25660290	0.75976502
C	-6.52769808	-0.44927635	1.84239400
C	-9.28008811	-0.71966405	1.45593300
H	-9.07788394	0.93816397	0.08302305
C	-7.24629718	-1.39819629	2.56133197
H	-5.46239707	-0.33698946	1.99838200
C	-8.61827820	-1.54909614	2.36062197
H	-10.34936712	-0.82081793	1.30629000
H	-6.72943025	-2.02717137	3.27731595
H	-9.16961628	-2.29835910	2.91718895
C	-1.23172958	4.44596925	-3.02687386
C	-1.06539166	3.76583027	-4.23830088
C	-2.38741060	4.24644235	-2.26613787
C	-2.03948975	2.86685138	-4.65936391
H	-0.18382564	3.94485319	-4.84146588
C	-3.33607670	3.31284946	-2.67105389
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H	-1.91056181	2.34120240	-5.59905292
H	-4.20227372	3.11897053	-2.04834690
H	-3.90692885	1.90248856	-4.19286593
C	1.47068548	4.89750278	3.04696915

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C	5.90657671	-3.40353153	0.46982103
C	7.64813567	-4.03508164	2.55164602
H	5.97443572	-3.63128947	3.85745104
C	7.21990967	-3.76891065	0.18823902
H	5.21334072	-3.16088349	-0.32588797
C	8.09321366	-4.08394971	1.22669302
H	8.33026166	-4.27717569	3.35987002
H	7.55487866	-3.80299570	-0.84202398
H	9.11827863	-4.36444380	1.00957501
Cl	-1.63720302	-0.18390189	-0.04024595

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H	3.02320339	4.01900958	4.25673412
C	2.14372655	5.65352378	0.85201017
H	0.15919458	5.88769896	1.67234218
C	3.44405950	5.21468364	1.10128115
H	4.77353141	4.31294845	2.53448112
H	1.89135859	6.09589783	-0.10492782
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C	-5.78418303	-1.49382489	-0.10156801
C	-5.80886602	-0.89576591	1.14888299
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H	-5.80091298	1.36640213	-1.98595498
H	-5.69684404	-2.56070989	-0.24334202
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O	-5.71534602	-1.35798187	-2.42587201
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O	-5.77228304	-1.58192892	2.33448099
C	-5.84476106	-3.00108592	2.32853397
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C	-5.78588200	-0.64788685	-3.65503300
H	-6.53171999	0.15326116	-3.59278600
H	-6.14704501	-1.37005184	-4.38952301
C	-5.98366797	3.36066609	1.37308804
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C	-4.46574199	-0.11373887	-4.13232199
C	-3.27905699	0.11020711	-3.47871199
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C	-1.11792908	-4.43958197	1.42204297
C	-0.46409809	-5.65778299	1.67424596
C	-0.43212406	-3.37071098	0.84362999
C	0.86947091	-5.80288400	1.34526397
H	-1.02211411	-6.46713998	2.12258595
C	0.90877494	-3.52991399	0.51890499
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C	-5.65454407	-0.07153277	-1.63711699
C	-5.13469508	-1.15831669	-2.35459813
C	-4.92211210	-2.35581078	-1.68918427
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H	-6.30852005	0.65472700	0.30374710
H	-4.87535609	-1.00133457	-3.39086411
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H	-6.88560603	2.74854637	-2.65474964
C	-5.88276608	-2.58569527	2.45657170
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C	-4.05331612	-3.48698755	-3.64403141
H	-4.76129611	-2.88857747	-4.22749934
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C	-2.63619111	-3.06083854	-3.89773837
C	-1.76773810	-2.28675264	-3.16772828
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C	-4.30264202	2.92489908	-0.53283363
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C	-2.64978798	5.87531086	1.06359572
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H	-3.42138297	6.58603490	0.80493581
C	-0.50261998	5.34230171	2.04965964

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C	-0.44413598	1.01831407	-3.12590697
C	0.91803804	1.75284907	-5.44716795
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C	0.87900702	1.41754605	-3.05338296
H	-0.95639799	0.73189606	-2.21172997
C	1.57583603	1.79165705	-4.21197795
H	1.47001204	2.04162707	-6.33370995
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C	0.90329102	2.59898199	2.43184206
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C	1.81952192	-2.76348549	3.49496065
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C	0.27546028	-5.51047196	-0.69945797
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O	0.70681669	-3.82514723	-3.76041777
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H	-2.53952272	4.42996461	-1.85060842
C	-2.08962785	2.78228264	-4.77796389
H	-0.39528084	3.01452310	-6.07208197
H	-3.65185684	2.76738222	-3.30729488
H	-2.57792190	2.05858547	-5.41784065
C	2.67836725	3.69810906	3.76707580
C	3.65302419	2.87654517	4.32358106
C	2.86488328	4.24832564	2.50302362
C	4.79659017	2.58239886	3.59814315
H	3.51725517	2.47298150	5.31837419
C	4.00547126	3.93866533	1.78056571
H	2.11052833	4.90564556	2.08926341
C	4.97178720	3.10519544	2.32574998
H	5.55350913	1.93926794	4.02914235
H	4.14178828	4.35219700	0.78915158
H	5.86308118	2.86657119	1.75982905
Br	0.62986790	-1.06107108	-0.22742666

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